Volume 69B
Number 4
Oct.–Dec. 1965

Mathematics and Mathematical Physics

U.S. DEPARTMENT OF COMMERCE

SECTION B

JOURNAL OF RESEARCH

NATIONAL BUREAU OF STANDARDS

Journal of Research

of the

National Bureau of Standards

B. Mathematics and Mathematical Physics

OCT.–DEC. • 1965

VOLUME • 69B

NUMBER • 4

Editor: Chester H. Page

Associate Editor: John J. Sopka

Publication dates: Mar. 10, June 10, Sept. 10, Dec. 10, 1965

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Use of funds for printing this publication approved by the Director of the Bureau of the Budget (June 19, 1961).

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 69B, No. 4, October–December 1965

Table of Dedekind Sums [1]

R. Dale Shipp [2]

(June 17, 1965)

The Dedekind sums are of importance in the transformation formulae for the Dedekind modular form $\eta(\tau)$, and in discussing the characters of degree 1 of the modular group and its subgroups. These sums are rational numbers and a table of their exact values is given. In addition a comprehensive bibliography on these sums is included.

Key Words: Dedekind sums, tables, characters, modular form.

1. Introduction

The purpose of this paper is to present a short table of Dedekind sums $s(h, k)$. These sums arise in the theory of modular forms and in number theory as well as in various other areas of mathematics. We have included a fairly extensive bibliography.[3]

In order to define a Dedekind sum, we first introduce the following symbol:

$$((x)) = x - [x] - \tfrac{1}{2} \quad \text{for } x \text{ not an integer}$$
$$= 0 \quad \text{for } x \text{ an integer} \tag{1.1}$$

where $[x]$ denotes the greatest integer not exceeding x. Then a Dedekind sum is defined by

$$s(h, k) = \sum_{u=1}^{k} ((hu/k))((u/k)) \tag{1.2}$$

where h is any integer and k is any positive integer.

The paper of Rademacher and Whiteman [1941], contains a number of interesting theorems on Dedekind sums. A later paper by Rademacher [1956], extends some of these results. In section 2 we quote some of these theorems. The interested reader is referred to these papers for proofs.

2. Theorems on Dedekind Sums

In this paragraph we present, without proof, theorems on Dedekind sums which will be helpful in using and extending the table.

THEOREM 1. *For integers* h, q, k, *with* q *and* k *positive* s(qh, qk) = s(h, k). [**RW**, p. 380].

This theorem allows us to consider only $(h, k) = 1$. In fact, Rademacher in [**R**] places this restriction on the definition of $s(h, k)$.

THEOREM 2. *If* $h_1 \equiv h_2$ *mod* k *then* $s(h_1, k) = s(h_2, k)$. [**R**, p. 445].

THEOREM 3. $s(-h, k) = -s(h, k)$. [**R**, p. 445].

Theorems 1, 2, and 3 allow us to obtain $s(h, k)$ for all h and for all k less than some fixed limit K from a table giving $s(h, k)$ only for $k = 2, 3, \ldots, K$ and h each integer in the interval $[1, [k/2]]$ such that $(h, k) = 1$.

THEOREM 4. *If* $h_1 h_2 \equiv 1$ *mod* k *then* $s(h_1, k) = s(h_2, k)$ [**R**, p. 445].

THEOREM 5. *The denominator of* s(h, k) *is at most* $2k \cdot (3, k)$ *where* (n, m) *denotes the greatest common divisor of* n *and* m [**R**, p. 446].

The main theorem on Dedekind sums is the following reciprocity relation.

THEOREM 6. *If* $h > 0$, $k > 0$, $(h, k) = 1$ *then*

$$s(h, k) + s(k, h) = -\frac{1}{4} + (h/k + k/h + 1/hk)/12.$$

There are many proofs of this theorem (e.g. [**RW**, p. 381], [**R**, p. 445]). In computing our table we used the reciprocity relation for Dedekind sums. It allows the computation of $s(h_0, k_0)$ using a table of $s(h, k)$ for $k < k_0$ without directly computing the sum in the definition. This relation will also be quite useful to the reader who wishes values of $s(h, k)$ not in the table. For example, if $1 \leq h \leq 100$ then $s(h, k)$ can be obtained for any $k > 0$ by at most one application of the reciprocity formula.

3. Authentication and Description of Computing Procedures

The program was written in FORTRAN 60 and run on a CDC 1604 computer. After using a sieve type method to eliminate from consideration those h except for $1 \leq h \leq [k/2]$ and $(h, k) = 1$, $s(h, k)$ was computed (in rational form) by using the reciprocity relation. It was then reduced until the numerator and denominator were without common factor and entered into the table. This table remained in storage until computation was completed at which time it was punched on cards. The punched cards were then printed using an IBM 407 accounting machine.

This table was checked visually with another unpublished table (computed by Robert A. Tobey using (1.2) directly) and the two were found to be in complete agreement.

[1] This project was sponsored by Wisconsin Alumni Research Funds.
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[3] The author wishes to acknowledge appreciation to Professor J. R. Smart for his assistance in the preparation of this paper.

k	h	s(h, k)	k	h	s(h, k)	k	h	s(h, k)	k	h	s(h, k)	k	h	s(h, k)	k	h	s(h, k)
2	1	0/1	23	6	17/46	32	13	19/64	40	9	23/80	46	13	−11/46	51	22	91/306
3	1	1/18	23	7	−1/46	32	15	−27/64	40	11	17/80	46	15	−45/46	51	23	−55/306
4	1	1/8	23	8	21/46	33	1	248/99	40	13	−13/16	46	17	3/46	51	25	−575/306
5	1	1/5	23	9	−7/46	33	2	112/99	40	17	−5/16	46	19	3/46	52	1	425/104
5	2	0/1	23	10	−1/46	33	4	32/99	40	19	−47/80	46	21	−5/46	52	3	119/104
6	1	5/18	23	11	−33/46	33	5	31/99	41	1	130/41	47	1	345/94	52	5	5/8
7	1	5/14	24	1	253/144	33	7	23/99	41	2	60/41	47	2	161/94	52	7	47/104
7	2	1/14	24	5	53/144	33	8	−32/99	41	3	39/41	47	3	105/94	52	9	41/104
7	3	−1/14	24	7	19/144	33	10	5/99	41	4	20/41	47	4	81/94	52	11	31/104
8	1	7/16	24	11	−37/144	33	13	−31/99	41	5	10/41	47	5	51/94	52	15	47/104
8	3	1/16	25	1	**46/25**	33	14	−23/99	41	6	25/41	47	6	65/94	52	17	−119/104
9	1	14/27	25	2	**4/5**	33	16	−112/99	41	7	25/41	47	7	37/94	52	19	31/104
9	2	4/27	25	3	2/5	34	1	44/17	41	8	−10/41	47	8	65/94	52	21	5/8
9	4	−4/27	25	4	4/25	34	3	11/17	41	9	0/1	47	9	5/94	52	23	−41/104
10	1	3/5	25	6	−4/25	34	5	9/17	41	10	−20/41	47	10	15/94	52	25	−87/104
10	3	0/1	25	7	0/1	34	7	9/17	41	11	9/41	47	11	−1/94	53	1	221/53
11	1	15/22	25	8	−2/5	34	9	4/17	41	12	3/41	47	12	81/94	53	2	104/53
11	2	5/22	25	9	4/25	34	11	−11/17	41	13	−11/41	47	13	7/94	53	3	68/53
11	3	3/22	25	11	−4/25	34	13	0/1	41	14	39/41	47	14	−15/94	53	4	39/53
11	4	3/22	25	12	−4/5	34	15	−4/17	41	15	9/41	47	15	−33/94	53	5	34/53
11	5	−5/22	26	1	25/13	35	1	187/70	41	16	−4/41	47	16	**105/94**	53	6	41/53
12	1	55/72	26	3	7/13	35	2	17/14	41	17	−3/41	47	17	1/94	53	7	17/53
12	5	−1/72	26	5	0/1	35	3	11/14	41	18	−4/41	47	18	−7/94	53	8	20/53
13	1	11/13	26	7	2/13	35	4	43/70	41	19	−11/41	47	19	51/94	53	9	41/53
13	2	4/13	26	9	7/13	35	6	37/70	41	20	−60/41	47	20	−37/94	53	10	11/53
13	3	1/13	26	11	−2/13	35	8	1/14	42	1	205/63	47	21	5/94	53	11	21/53
13	4	−1/13	27	1	325/162	35	9	43/70	42	5	29/63	47	22	−33/94	53	12	8/53
13	5	0/1	27	2	143/162	35	11	−13/70	42	11	20/63	47	23	−161/94	53	13	−39/53
13	6	−4/13	27	4	73/162	35	12	11/14	42	13	−2/63	48	1	1081/288	53	14	16/53
14	1	13/14	27	5	35/162	35	13	−1/14	42	17	29/63	48	5	161/288	53	15	−17/53
14	3	3/14	27	7	73/162	**35**	16	−13/70	42	19	−20/63	48	7	199/288	53	16	11/53
14	5	3/14	27	8	−1/162	**35**	17	−17/14	43	1	287/86	48	11	−1/288	53	17	−23/53
15	1	91/90	27	10	1/162	**36**	1	595/216	43	2	133/86	48	13	1/288	53	18	68/53
15	2	7/18	27	11	35/162	**36**	5	35/216	43	3	77/86	48	17	89/288	53	19	16/53
15	4	19/90	27	13	−143/162	**36**	7	−35/216	43	4	67/86	48	19	−161/288	53	20	20/53
17					117/56	36	11	−19/216	43	5	41/86	48	23	−217/288	53	21	−34/53
16					27/56	36	13	19/216	43	6	7/86	49	1	188/49	53	22	−8/53
16					13/56	36	17	−109/216	43	7	−7/86	49	2	88/49	53	23	0/1
16					−27/56	37	1	105/37	43	8	13/86	49	3	52/49	53	24	−21/53
16					−13/56	37	2	48/37	43	9	27/86	49	4	32/49	53	25	−23/53
17	1	20/17	28	13	−19/56	37	3	27/37	43	10	11/86	49	5	38/49	53	26	−104/53
17	2	8/17	29	1	63/29	37	4	15/37	43	11	67/86	49	6	8/49	54	1	689/162
17	3	5/17	29	2	28/29	37	5	14/37	43	12	5/86	49	8	−8/49	54	5	139/162
17	4	0/1	29	3	18/29	37	6	0/1	43	13	11/86	49	9	18/49	54	7	77/162
17	5	1/17	29	4	7/29	37	7	5/37	43	14	−77/86	49	10	38/49	54	11	139/162
17	6	5/17	29	5	13/29	37	8	8/37	43	15	35/86	49	11	18/49	54	13	−31/162
17	7	1/17	29	6	13/29	37	9	−15/37	43	16	−13/86	49	12	−32/49	54	17	−41/162
17	8	−8/17	29	7	−7/29	37	10	3/37	43	17	−41/86	49	13	8/49	54	19	41/162
18	1	34/27	29	8	4/29	37	11	−3/37	43	18	5/86	49	15	−8/49	54	23	−77/162
18	5	2/27	29	9	−3/29	37	12	−27/37	43	19	−27/86	49	16	−52/49	54	25	−31/162
18	7	−2/27	29	10	18/29	37	13	12/37	43	20	−35/86	49	17	24/49	55	1	477/110
19	1	51/38	29	11	4/29	37	14	8/37	43	21	−133/86	49	18	4/49	55	2	45/22
19	2	21/38	29	12	0/1	37	15	14/37	44	1	301/88	49	19	−4/49	55	3	27/22
19	3	9/38	29	13	−3/29	37	16	5/37	44	3	91/88	49	20	8/49	55	4	113/110
19	4	11/38	29	14	−28/29	37	17	−12/37	44	5	61/88	49	22	−8/49	55	6	27/110
19	5	11/38	30	1	203/90	37	18	−48/37	44	7	19/88	49	23	−24/49	55	7	17/22
19	6	−9/38	30	7	1/18	38	1	111/38	44	9	61/88	49	24	−88/49	55	8	17/22
19	7	3/38	30	11	13/90	38	3	33/38	44	13	5/88	50	1	98/25	55	9	−27/110
19	8	−3/38	30	13	1/18	38	5	15/38	44	15	91/88	50	3	6/5	55	12	3/22
19	9	−21/38	31	1	145/62	38	7	11/38	44	17	5/88	50	7	0/1	55	13	1/22
20	1	57/40	**31**	**2**	**65/62**	38	9	−1/38	44	19	19/88	50	9	2/25	55	14	113/110
20	3	3/8	**31**	**3**	**35/62**	38	11	11/38	44	21	−59/88	50	11	−2/25	55	16	17/110
20	7	3/8	**31**	**4**	**33/62**	38	13	33/38	45	1	473/135	50	13	2/5	55	17	1/22
20	9	−7/40	**31**	**5**	**5/62**	38	15	−15/38	45	2	44/27	50	17	6/5	55	18	−27/22
21	1	95/63	**31**	**6**	**−5/62**	38	17	−1/38	45	4	77/135	50	19	2/25	55	19	63/110
21	2	40/63	31	7	13/62	39	1	703/234	45	7	10/27	50	21	−2/25	55	21	7/110
21	4	5/63	31	8	33/62	39	2	323/234	45	8	8/27	50	23	−2/5	55	23	3/22
21	5	−5/63	31	9	13/62	39	4	163/234	45	11	−77/135	51	1	1225/306	55	24	−17/110
21	8	4/63	31	10	−35/62	39	5	11/18	45	13	10/27	51	2	575/306	55	26	−63/110
21	10	−40/63	31	11	15/62	39	7	37/234	45	14	−23/135	51	4	17/18	55	27	−45/22
22	1	35/22	31	12	−1/62	39	8	11/18	45	16	23/135	51	5	125/306	56	1	495/112
22	3	7/22	31	13	−1/62	39	10	163/234	45	17	8/27	51	7	91/306	56	3	153/112
22	5	3/22	31	14	−15/62	39	11	−37/234	45	19	−13/135	51	8	71/306	56	5	55/112
22	7	−7/22	31	15	−65/62	39	14	53/234	45	22	−44/27	51	10	−125/306	56	9	15/112
22	9	3/22	32	1	155/64	39	16	19/234	46	1	165/46	51	11	89/306	56	11	−55/112
23	1	77/46	32	3	45/64	39	17	−19/234	46	3	45/46	51	13	17/18	56	13	23/112
23	2	33/46	32	5	19/64	39	19	−323/234	46	5	15/46	51	14	89/306	56	15	33/112
23	3	21/46	32	7	5/64	40	1	247/80	46	7	11/46	51	16	−35/306	56	17	−1/112
23	4	17/46	32	9	−5/64	40	3	13/16	46	9	−15/46	51	19	−71/306	56	19	153/112
23	5	7/46	32	11	45/64	40	7	5/16	46	11	−5/46	51	20	−55/306	56	23	1/112

k	h	s(h, k)	k	h	s(h, k)	k	h	s(h, k)
56	25	15/112	61	10	−20/61	65	14	24/65
56	27	−103/112	61	11	0/1	65	16	−64/65
57	1	770/171	61	12	−35/61	65	17	5/13
57	2	364/171	61	13	5/61	65	18	0/1
57	4	140/171	61	14	−5/61	65	19	9/65
57	5	121/171	61	15	−55/61	65	21	−3/5
57	7	14/171	61	16	15/61	65	22	21/13
57	8	−14/171	61	17	8/61	65	23	5/13
57	10	41/171	61	18	8/61	65	24	9/65
57	11	−5/171	61	19	−15/61	65	27	−3/13
57	13	23/171	61	20	−85/61	65	28	6/13
57	14	−140/171	61	21	40/61	65	29	14/65
57	16	−4/171	61	22	9/61	65	31	−3/5
57	17	−41/171	61	23	28/61	65	32	−32/13
57	20	67/171	61	24	−16/61	66	1	520/99
57	22	23/171	61	25	9/61	66	5	65/99
57	23	121/171	61	26	−34/61	66	7	61/99
57	25	−4/171	61	27	−29/61	66	13	−65/99
57	26	−5/171	61	28	−16/61	66	17	56/99
57	28	−364/171	61	29	−40/61	66	19	61/99
58	1	133/29	61	30	−140/61	66	23	47/99
58	3	38/29	62	1	305/62	66	25	16/99
58	5	21/29	62	3	95/62	66	29	−16/99
58	7	11/29	62	5	49/62	66	31	−56/99
58	9	13/29	62	7	53/62	67	1	715/134
58	11	2/29	62	9	53/62	67	2	341/134
58	13	13/29	62	11	23/62	67	3	209/134
58	15	14/29	62	13	15/62	67	4	171/134
58	17	0/1	62	15	−17/62	67	5	117/134
58	19	−38/29	62	17	23/62	67	6	55/134
58	21	−2/29	62	19	−15/62	67	7	65/134
58	23	−21/29	62	21	95/62	67	8	53/134
58	25	11/29	62	23	−1/62	67	9	71/134
58	27	−14/29	62	25	49/62	67	10	43/134
59	1	551/118	62	27	−1/62	67	11	−55/134
59	2	261/118	62	29	−17/62	67	12	29/134
59	3	171/118	63	1	1891/378	67	13	−15/134
59	4	131/118	63	2	899/378	67	14	51/134
59	5	111/118	63	4	451/378	67	15	71/134
59	6	101/118	63	5	305/378	67	16	−5/134
59	7	63/118	63	8	323/378	67	17	171/134
59	8	37/118	63	10	109/378	67	18	21/134
59	9	19/118	63	11	143/378	67	19	−65/134
59	10	101/118	63	13	181/378	67	20	−43/134
59	11	9/118	63	16	451/378	67	21	−5/134
59	12	111/118	63	17	53/378	67	22	−209/134
59	13	−19/118	63	19	109/378	67	23	99/134
59	14	−11/118	63	20	−127/378	67	24	51/134
59	15	131/118	63	22	127/378	67	25	−53/134
59	16	−9/118	63	23	143/378	67	26	−21/134
59	17	63/118	63	25	−305/378	67	27	117/134
59	18	−3/118	63	26	53/378	67	28	29/134
59	19	−61/118	63	29	−181/378	67	29	11/134
59	20	171/118	63	31	−899/378	67	30	−11/134
59	21	11/118	64	1	651/128	67	31	−15/134
59	22	−37/118	64	3	189/128	67	32	−99/134
59	23	−3/118	64	5	131/128	67	33	−341/134
59	24	29/118	64	7	21/128	68	1	737/136
59	25	−21/118	64	9	−21/128	68	3	231/136
59	26	−21/118	64	11	61/128	68	5	121/136
59	27	−29/118	64	13	131/128	68	7	87/136
59	28	−61/118	64	15	−11/128	68	9	33/136
59	29	−261/118	64	17	11/128	68	11	7/136
60	1	1711/360	64	19	−3/128	68	13	1/8
60	7	29/72	64	21	−189/128	68	15	−33/136
60	11	161/360	64	23	21/128	68	19	−1/136
60	13	11/72	64	25	−21/128	68	21	1/8
60	17	−29/72	64	27	−3/128	68	23	231/136
60	19	−71/360	64	29	−61/128	68	25	1/136
60	23	−11/72	64	31	−139/128	68	27	−121/136
60	29	−361/360	65	1	336/65	68	29	−87/136
61	1	295/61	65	2	32/13	68	31	7/136
61	2	140/61	65	3	21/13	68	33	−159/136
61	3	85/61	65	4	64/65	69	1	1139/207
61	4	55/61	65	6	61/65	69	2	544/207
61	5	35/61	65	7	6/13	69	4	221/207
61	6	20/61	65	8	0/1	69	5	229/207
61	7	34/61	65	9	14/65	69	7	194/207
61	8	28/61	65	11	61/65	69	8	112/207
61	9	29/61	65	12	3/13	69	10	194/207
69	11	31/207	73	7	51/73	76	27	35/152
69	13	59/207	73	8	6/73	76	29	21/152
69	14	229/207	73	9	−6/73	76	31	35/152
69	16	59/207	73	10	27/73	76	33	−11/152
69	17	−221/207	73	11	33/73	76	35	−85/152
69	19	32/207	73	12	−36/73	76	37	−203/152
69	20	49/207	73	13	17/73	77	1	475/77
69	22	−58/207	73	14	−1/73	77	2	228/77
69	25	−31/207	73	15	41/73	77	3	150/77
69	26	112/207	73	16	4/73	77	4	95/77
69	28	68/207	73	17	5/73	77	5	80/77
69	29	−32/207	73	18	−84/73	77	6	85/77
69	31	−49/207	73	19	24/73	77	8	48/77
69	32	−68/207	73	20	33/73	77	9	25/77
69	34	−544/207	73	21	51/73	77	10	31/77
70	1	391/70	73	22	27/73	77	12	24/77
70	3	23/14	73	23	−24/73	77	13	85/77
70	9	39/70	73	24	−126/73	77	15	−15/77
70	11	11/70	73	25	60/73	77	16	25/77
70	13	3/14	73	26	1/73	77	17	−25/77
70	17	−5/14	73	27	0/1	77	18	4/77
70	19	−11/70	73	28	−17/73	77	19	−95/77
70	23	−23/14	73	29	−71/73	77	20	36/77
70	27	3/14	73	30	−5/73	77	23	−31/77
70	29	−1/70	73	31	−19/73	77	24	−25/77
70	31	−39/70	73	32	4/73	77	25	−59/77
70	33	−5/14	73	33	−19/73	77	26	150/77
71	1	805/142	73	34	−41/73	77	27	36/77
71	2	385/142	73	35	−60/73	77	29	48/77
71	3	253/142	73	36	−204/73	77	30	4/77
71	4	193/142	74	1	219/37	77	31	80/77
71	5	105/142	74	3	69/37	77	32	−24/77
71	6	145/142	74	5	44/37	77	34	−20/77
71	7	35/142	74	7	21/37	77	36	−15/77
71	8	133/142	74	9	11/37	77	37	−59/77
71	9	133/142	74	11	17/37	77	38	−228/77
71	10	−35/142	74	13	6/37	78	1	1463/234
71	11	75/142	74	15	44/37	78	5	19/18
71	12	145/142	74	17	−6/37	78	7	77/234
71	13	75/142	74	19	24/37	78	11	−77/234
71	14	−105/142	74	21	−21/37	78	17	49/234
71	15	53/142	74	23	−4/37	78	19	−103/234
71	16	33/142	74	25	69/37	78	23	49/234
71	17	−25/142	74	27	17/37	78	25	−85/234
71	18	193/142	74	29	−4/37	78	29	−23/234
71	19	53/142	74	31	0/1	78	31	−19/18
71	20	−15/142	74	33	11/37	78	35	−23/234
71	21	−1/142	74	35	−24/37	78	37	−103/234
71	22	−13/142	75	1	2701/450	79	1	1001/158
71	23	−97/142	75	2	259/90	79	2	481/158
71	24	253/142	75	4	649/450	79	3	299/158
71	25	25/142	75	7	13/18	79	4	241/158
71	26	23/142	75	8	43/90	79	5	201/158
71	27	1/142	75	11	251/450	79	6	91/158
71	28	−49/142	75	13	29/90	79	7	99/158
71	29	13/142	75	14	−1/450	79	8	161/158
71	30	−23/142	75	16	1/450	79	9	101/158
71	31	−33/142	75	17	7/90	79	10	161/158
71	32	−15/142	75	19	649/450	79	11	21/158
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71	34	−97/142	75	23	−29/90	79	13	−91/158
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72	1	2485/432	75	28	−43/90	79	15	−1/158
72	5	413/432	75	29	−1/450	79	16	201/158
72	7	235/432	75	31	1/450	79	17	71/158
72	11	35/432	75	32	−13/18	79	18	33/158
72	13	−35/432	75	34	−251/450	79	19	−19/158
72	17	53/432	75	37	−259/90	79	20	241/158
72	19	163/432	76	1	925/152	79	21	1/158
72	23	−181/432	76	3	275/152	79	22	33/158
72	25	181/432	76	5	125/152	79	23	13/158
72	29	413/432	76	7	155/152	79	24	−13/158
72	31	235/432	76	9	93/152	79	25	−19/158
72	35	−541/432	76	11	155/152	79	26	−299/158
73	1	426/73	76	13	85/152	79	27	143/158
73	2	204/73	76	15	−125/152	79	28	39/158
73	3	126/73	76	17	93/152	79	29	23/158
73	4	84/73	76	21	21/152	79	30	23/158
73	5	**71/73**	76	23	11/152	79	31	−39/158
73	6	36/73	76	25	−275/152	79	32	65/158

k	h	s(h, k)
79	33	47/158
79	34	99/158
79	35	−101/158
79	36	21/158
79	37	−65/158
79	38	−143/158
79	39	−481/158
80	1	1027/160
80	3	65/32
80	7	25/32
80	9	163/160
80	11	37/160
80	13	−1/32
80	17	7/32
80	19	−27/160
80	21	27/160
80	23	25/32
80	27	65/32
80	29	−37/160
80	31	−3/160
80	**33**	7/32
80	37	−1/32
80	39	−227/160
81	1	1580/243
81	2	760/243
81	4	320/243
81	5	220/243
81	7	158/243
81	8	40/243
81	10	−40/243
81	11	58/243
81	13	50/243
81	14	112/243
81	16	−220/243
81	17	40/243
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81	22	−58/243
81	23	−158/243
81	25	50/243
81	26	−122/243
81	28	122/243
81	29	112/243
81	31	−4/243
81	32	−104/243
81	34	−4/243
81	35	40/243
81	37	−40/243
81	38	−104/243
81	40	−760/243
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82	39	−30/41
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83	6	197/166
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83	17	107/166
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83	19	9/166
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83	28	351/166
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83	30	11/166
83	31	−93/166
83	32	99/166
83	33	−189/166
83	34	37/166
83	35	9/166
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83	37	63/166
83	38	−53/166
83	39	−107/166
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84	17	**683/504**
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84	31	109/504
84	37	−53/504
84	41	−757/504
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85	14	−56/85
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85	18	4/17
85	19	59/85
85	21	−7/5
85	22	7/17
85	23	1/17
85	24	−16/85
85	26	−9/85
85	27	−7/17
85	28	−35/17
85	29	84/85
85	31	46/85
85	32	12/17
85	33	−4/17
85	36	−9/85
85	37	1/17
85	38	0/1
85	39	−16/85
85	41	−84/85
85	42	−56/17
86	1	595/86
86	3	189/86
86	5	85/86
86	7	61/86
86	9	35/86
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86	39	−55/86
86	41	−45/86
87	1	3655/522
87	2	1763/522
87	4	883/522
87	5	**629/522**
87	7	451/522
87	8	575/522
87	10	253/522
87	11	575/522
87	13	127/522
87	14	35/522
87	16	163/522
87	17	−5/18
87	19	37/522
87	20	−127/522
87	22	883/522
87	23	125/522
87	25	451/522
87	26	−253/522
87	28	−233/522
87	31	−35/522
87	32	−37/522
87	34	−125/522
87	35	629/522
87	37	−179/522
87	38	−163/522
87	40	−179/522
87	41	−5/18
87	43	−1763/522
88	1	1247/176
88	3	377/176
88	5	215/176
88	7	129/176
88	9	127/176
88	13	71/176
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88	19	41/176
88	21	7/176
88	23	81/176
88	25	−129/176
88	27	−71/176
88	29	−377/176
88	31	17/176
88	35	−215/176
88	37	−41/176
88	39	−127/176
88	41	−113/176
88	43	−279/176
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89	3	203/89
89	4	132/89
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89	15	113/89
89	16	12/89
89	17	18/89
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89	24	19/89
89	25	−8/89
89	26	19/89
89	27	5/89
89	28	−17/89
89	29	−83/89
89	30	203/89
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89	33	5/89
89	34	0/1
89	35	−17/89
89	36	44/89
89	37	−35/89
89	38	−79/89
89	39	12/89
89	40	−28/89
89	41	−57/89
89	42	−44/89
89	43	−83/89
89	44	−308/89
90	1	979/135
90	7	32/27
90	11	29/135
90	13	32/27
90	17	4/27
90	19	61/135
90	23	22/27
90	29	−79/135
90	31	79/135
90	37	−4/27
90	41	29/135
90	43	−22/27
91	1	1335/182
91	2	645/182
91	3	405/182
91	4	323/182
91	5	15/14
91	6	135/182
91	8	9/14
91	9	15/182
91	10	−15/182
91	11	57/182
91	12	69/182
91	15	−135/182
91	16	15/182
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91	18	−15/14
91	19	83/182
91	20	−5/182
91	22	−37/182
91	23	323/182
91	24	83/182
91	25	43/182
91	27	9/182
91	29	−37/182
91	30	−405/182
91	31	15/14
91	32	57/182
91	33	−57/182
91	34	−9/14
91	36	−93/182
91	37	57/182
91	38	69/182
91	40	−43/182
91	41	−5/182
91	43	−93/182
91	44	−15/14
91	45	−645/182
92	1	1365/184
92	3	435/184
92	5	237/184
92	7	91/184
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92	43	−21/184
92	45	−307/184
93	1	2093/279
93	2	1012/279
93	4	437/279
93	5	364/279
93	7	221/279
93	8	220/279
93	10	149/279
93	11	193/279
93	13	14/279
93	14	148/279
93	16	113/279
93	17	193/279
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93	29	−113/279
93	32	202/279
93	34	68/279
93	35	220/279
93	37	−364/279
93	38	4/279
93	40	221/279
93	41	−68/279
93	43	14/279
93	44	−203/279
93	46	−1012/279
94	1	713/94
94	3	217/94
94	5	143/94
94	7	89/94
94	9	73/94
94	11	23/94
94	13	27/94
94	15	7/94
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94	19	143/94
94	21	73/94
94	23	−57/94
94	25	−7/94
94	27	89/94
94	29	27/94
94	31	−217/94
94	33	31/94
94	35	−17/94
94	37	−31/94
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94	41	−9/94
94	43	−17/94
94	45	−57/94
95	1	1457/190
95	2	141/38
95	3	93/38
95	4	353/190
95	6	257/190
95	7	31/38
95	8	45/38
95	9	93/190
95	11	117/190
95	12	45/38
95	13	17/38
95	14	103/190
95	16	257/190
95	17	11/38
95	18	5/38
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95	23	−13/38
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95	26	117/190
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95	34	103/190
95	36	17/190
95	37	5/38
95	39	13/190
95	41	47/190
95	42	−13/38
95	43	−13/38
95	44	−47/190
95	46	−193/190
95	47	−141/38
96	1	4465/576
96	5	665/576
96	7	559/576
96	11	359/576
96	13	217/576
96	17	305/576
96	19	−665/576
96	23	−145/576
96	25	145/576
96	29	89/576
96	31	−305/576
96	35	359/576
96	37	217/576
96	41	−559/576
96	43	−89/576
96	47	−1009/576
97	1	760/97
97	2	368/97
97	3	232/97
97	4	160/97
97	5	133/97
97	6	80/97
97	7	123/97
97	8	32/97
97	9	78/97
97	10	55/97
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97	22	0/1
97	23	−3/97
97	24	−160/97
97	25	48/97
97	26	23/97
97	27	28/97
97	28	39/97
97	29	−55/97
97	30	−1/97
97	31	−48/97
97	32	−232/97
97	33	112/97
97	34	53/97
97	35	8/97
97	36	−8/97
97	37	21/97

k	h	$s(h,k)$	k	h	$s(h,k)$	k	h	$s(h,k)$
97	38	−3/97	98	45	−16/49	99	46	−161/594
97	39	133/97	98	47	−44/49	99	47	−343/594
97	40	29/97	99	1	4753/594	99	49	−2303/594
97	41	−23/97	99	2	2303/594	100	1	1617/200
97	42	1/97	99	4	1153/594	100	3	99/40
97	43	−78/97	99	5	953/594	100	7	7/8
97	44	−70/97	99	7	343/594	100	9	33/200
97	45	−39/97	99	8	431/594	100	11	−33/200
97	46	−35/97	99	10	703/594	100	13	13/40
97	47	−112/97	99	13	235/594	100	17	29/40
97	48	−368/97	99	14	−343/594	100	19	−17/200
98	1	388/49	99	16	73/594	100	21	17/200
98	3	124/49	99	17	323/594	100	23	−13/40
98	5	68/49	99	19	−53/594	100	27	3/40
98	9	58/49	99	20	953/594	100	29	33/200
98	11	58/49	99	23	89/594	100	31	−33/200
98	13	4/49	99	25	1153/594	100	33	−99/40
98	15	−4/49	99	26	53/594	100	37	−3/40
98	17	12/49	99	28	−161/594	100	39	−17/200
98	19	−2/49	99	29	35/594	100	41	17/200
98	23	−12/49	99	31	73/594	100	43	7/8
98	25	44/49	99	32	−397/594	100	47	−29/40
98	27	4/49	99	34	397/594	100	49	−367/200
98	29	−4/49	99	35	323/594			
98	31	−2/49	99	37	−431/594			
98	33	124/49	99	38	−235/594			
98	37	16/49	99	40	343/594			
98	39	−68/49	99	41	35/594			
98	41	4/49	99	43	−89/594			
98	43	−4/49	99	46	−161/594			

4. Bibliography

T. M. Apostol, Generalized Dedekind sums and transformation formulae of certain Lambert series, Duke Math. J. **17,** 147–157 (1950); MR **11,** 641.

T. M. Apostol, Theorems on generalized Dedekind sums, Pacific J. Math. **2,** 1–9 (1952); MR **13,** 725.

L. Carlitz, Some theorems on generalized Dedekind sums, Pacific J. Math. **3,** 513–522 (1953); MR **15,** 12.

L. Carlitz, The reciprocity theorem for Dedekind sums, Pacific J. Math. **3,** 523–527 (1953); MR **15,** 12.

R. Dedekind, Erlauterungen zu den vorstehenden Fragmenten, Riemann's Gesammelte Werke, pp. 466–478; Dedekind's Gesammelte Werke Bd **1,** 159–172 (1930).

R. Dedekind, Schreiben an Herr Borchardt uber die Theorie der elliptischen Modulfunktionen, J. Reine Angew. Math. **83,** 265–292 (1877); also Dedekind's Gesammelte Werke, Bd **1,** pp. 174–201.

U. Dieter, Beziehungen zwischen Dedekindschen Summen, Abh. Math. Sem. Univ. Hamburg. **21,** 109–125 (1957); MR **19,** 395.

C. Meyer, Uber enige Anwendungen Dedekindschen Summen, J. Reine Angew. Math. **198,** 143–203 (1957); MR **21, #**3396.

L. J. Mordell, Lattice points in a tetrahedron and generalized Dedekind sums, J. Indian Math. Soc. **15,** 41–46 (1951); MR **13,** 322.

L. J. Mordell, The reciprocity for Dedekind sums, Amer. J. Math. **73,** 593–598 (1951); MR **13,** 113.

Morris Newman, Construction and application of a class of modular functions. I, II, Proc. London Math. Soc. **7,** 334–350 (1957); MR **19,** 953; **9,** 373–387 (1959); MR **21, #**6354.

Hans Rademacher, Zur Theorie der Modulfunktionen, J. Reine Angew. Math. **167,** 312–336 (1931); Z **3,** 215.

Hans Rademacher, Bestimmung einer gewissen Einheitswurzel in der Theorie der Modulfunktionen, J. London Math. Soc. **7,** 14–19 (1932); Z **3,** 351.

Hans Rademacher, Ein arithmetische Summenformel, Monatsh. Math. Phys. **39,** 221–228 (1932).

Hans Rademacher, Uber eine Reziprozitatsformel aus der Theorie der Modulfunktionen, Mat. Fiz. Lap. **40,** 24–34, Z **8,** 75; FdM **59,** 1060.

Hans Rademacher, On the partition function $p(n)$, Proc. London Math. Soc. series 2, **43,** 241–254 (1937); Z **16,** 246.

Hans Rademacher, The Ramanujan identities under modular substitutions, Trans. Amer. Math. Soc. **51,** 609–636 (1942); MR **3,** 271.

Hans Rademacher, Die Reziprozitatsformel fur Dedekindsche Summen, Acta Sci. Math. (Szeged) **12B,** 57–60 (1950); MR **11,** 642.

Hans Rademacher, On Dedekind sums and lattice points in a tetrahedron, Studies in mathematics and mechanics presented to Richard von Mises (Academic Press, New York, 1954); pp. 49–53, MR **16,** 341.

Hans Rademacher, Generalization of the reciprocity formula for Dedekind sums, Duke Math. J. **21,** 1954, 391–397 (1954); MR **16,** 14.

Hans Rademacher, On the transformation of log $\eta(\tau)$, J. Indian Math. Soc. **19,** 25–30 (1955); MR **17,** 15.

Hans Rademacher, Zur Theorie der Dedekindschen Summen, Math. Z. **63,** 445–463 (1956); MR **18,** 114.

Hans Rademacher, Lectures on analytic number theory, Tata Institute of Fundamental Research, Bombay, 1954–55.

Hans Rademacher and A. L. Whitman, Theorems on Dedekind sums, Amer. J. Math. **63,** 377–407 (1941); MR **2,** 249.

L. Redei, Elementarer Beweis und Verallgemeinerung einer Reziprozitatsformel von Dedekind, Acta Sci. Math. (Szeged) **12B,** 236–239 (1950); MR **11,** 641.

Hans Salie, Zum Wertevorrat der Dedekindscher Summen, Math. Z. **72,** 61–75 (1959); MR **21, #**5601.

Klaus Wohlfahrt, Uber Dedekindsche Summen und Untergruppen der Modulgruppe, Abh. Math. Sem. Univ. Hamburg, **23,** 5–10 (1959); MR **21, #**1350.

(Paper 69B4–155)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 69B, No. 4, October–December 1965

Lattice Points in a Sphere

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(March 26, 1964)

Let $R_3(x)$ be the remainder in the classical lattice point problem for a 3-sphere of radius $\sqrt{x}$ and center (0, 0, 0). We prove that as $x \to +\infty$,

$$R_3(x) = O(x^{3/4} \log x)$$

and

$$R_3(x) = \Omega(x^{1/2} \log \log x).$$

Key Words: Additive analytic number theory, lattice points, remainder formulas.

1. Introduction

In this paper we consider the classical lattice point problem for the three-dimensional sphere. The problem can be described as follows. Let x be a positive real number and let k be a positive integer. Consider a k-dimensional sphere of radius $\sqrt{x}$ and center $(0, \ldots, 0)$. Following the notation of Walfisz [4],[2] we let $A_k(x)$ be the number of integer lattice points in this sphere. A simple geometric argument shows that as $x \to +\infty$, $A_k(x) \sim V_k(x)$, where $V_k(x)$ is the volume of the sphere in question. The problem then is to get an asymptotic estimate of the difference $R_k(x) = A_k(x) - V_k(x)$.

Here we are considering only $R_3(x) = A_3(x) - \frac{4}{3}\pi x^{3/2}$. We obtain the following results:

$$R_3(x) = O(x^{3/4} \log x), \; x \to +\infty \tag{1}$$

$$R_3(x) = \Omega(x^{1/2} \log \log x), \; x \to +\infty. \tag{2}$$

Of course (1) is not new. Vinogradov [3] has in fact shown that $R_3(x) = O(x^{\frac{19}{28}+\epsilon})$, $\epsilon > 0$, an upper estimate better than (1). However this result depends upon his difficult theory of exponential sums. Our estimate (1), on the other hand, is better than the elementary result $A_3(x) = O(x)$ and depends only upon a fairly standard application of the circle method.

As far as we can ascertain (2) is new. It is based upon the Ω-estimate for $R_4(x)$ [4, p. 95]

$$R_4(x) = \Omega(x \log \log x), \; x \to +\infty. \tag{3}$$

Walfisz [4, p. 94] gives only $R_3(x) = \Omega(x^{1/2})$, $x \to +\infty$. In [1] it is shown that $\lim_{x \to \infty} |R_3(x) x^{-1/2}| = +\infty$, but this is of course weaker than (3).

2. Preliminaries

Landau's formula for $A_k(x)$ $(k \geq 4)$ is [4, p. 29]

$$A_k(x) = \frac{\pi^{k/2}}{\Gamma\left(\frac{k}{2}\right)} \sum_{1 \leq q \leq x^{1/2}} {\sum_{h \pmod q}}' \left(\frac{S(h, q)}{q}\right)^k \cdot \sum_{1 \leq n \leq x} n^{k/2-1} e^{-2\pi i n h/q} + O(x^{k/4} \log x), \; x \to +\infty. \tag{4}$$

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[2] Figures in brackets indicate the literature references at the end of this paper.

Here $S(h, q)=\sum_{a(\mathrm{mod}\ q)} e^{2\pi i h a^2/q}$ is the famous Gaussian sum about which we need only the fact that

$$|S(h, q)| \leq Kq^{1/2}. \tag{5}$$

where K is independent of h and q [4, p. 10]. The notation Σ' indicates that we are to sum over only those h such that $(h, q)=1$.

If (4) held for $k=3$ we could apply it to derive (1) without much difficulty. However since the proof of (4) given in [4] fails for $k<4$, we replace it for $k=3$ with the following formula obtainable by the same general method.

$$A_3(x)=2\pi\sum_{n\leq x} n^{1/2}+O(x^{3/4}\log x),\ x\to+\infty. \tag{6}$$

Once we have (6), (1) is easily obtainable.

We will also need the following standard result [4, p. 25].

LEMMA 1 (*Euler Summation Formula*). *Let* $\Psi(t)=t-[t]-\frac{1}{2}$. *If* $f(t)$ *has a continuous derivative in the interval* $a\leq t\leq b (a<b)$, *then*

$$\sum_{a<m\leq b} f(m)=\int_a^b f(t)dt+\Psi(a)f(a)-\Psi(b)f(b)+\int_a^b \Psi(t)f'(t)dt. \tag{7}$$

This is proved by integrating $\int_a^b \Psi(t)f'(t)dt$ by parts.

3. Proof of (6) and (1)

Many of the calculations done in the proof of (4) [4, pp. 29–35] are valid for $k=3$. In particular we have [4, p. 33, formula (21)]

$$A_3(x)=\sum_{q\leq x^{1/2}}\sum_{h(\mathrm{mod}\ q)}{}' \left(\frac{S(h, q)}{q}\right)^3 \int_{\theta(h, q)} w^{-3/2} \sum_{n\leq x}\exp\left\{\frac{\pi n}{x}-2\pi i n\left(y+\frac{h}{q}\right)\right\}dy+O(x^{3/4}\log x),\ x\to+\infty. \tag{8}$$

In (8), $w=x^{-1}-2yi$, and $\theta(h, q)$ is an interval described as follows. Let h'/q' and h''/q'' be the two Farey fractions of order $x^{1/2}$ closest to h/q with say $h'/q'<h/q<h''/q''$, and consider the interval $\left[\frac{h'+h}{q'+q}, \frac{h+h''}{q+q''}\right]$. Then $\theta(h, q)$ is obtained from this interval by translating h/q to the origin, that is,

$$\theta(h, q)=\left[\frac{h'+h}{q'+q}-\frac{h}{q}, \frac{h+h''}{q+q''}-\frac{h}{q}\right].$$

For our purpose here the essential fact about $\theta(h, q)$ is [4, p. 30]

$$\begin{cases} |y|\leq q^{-1}x^{-1/2}, \text{ for } y\in\theta(h, q) \\ |y|\geq 2^{-1}q^{-1}x^{-1/2}, \text{ for } y\notin\theta(h, q). \end{cases} \tag{9}$$

for any Farey fraction h/q or order $x^{1/2}$.

By (8) we have

$$A_3(x)=\int_{\mathfrak{B}(0,\,1)} w^{-3/2}\sum_{n\le x}\exp\left\{\frac{\pi n}{x}-2\pi i n y\right\}dy$$

$$+\sum_{2\le q\le x^{1/2}}\sum_{h(\mathrm{mod}\ q)}{}'\left(\frac{S(h,\,q)}{q}\right)^3\int_{\mathfrak{B}(h,\,q)} w^{-3/2}\sum_{n\le x}\exp\left\{\frac{\pi n}{x}-2\pi i n\left(y+\frac{h}{q}\right)\right\}dy$$

$$+O(x^{3/4}\log x),\ x\to+\infty. \qquad (10)$$

Again we observe that the calculations of [4, pp. 33–34] are valid for $k=3$. These yield

$$\int_{\mathfrak{B}(0,\,1)} w^{-3/2}\sum_{n\le x}\exp\left\{\frac{\pi n}{x}-2\pi i n y\right\}dy=\int_{-\infty}^{\infty} w^{-3/2}\sum_{n\le x}\exp\left\{\frac{\pi n}{x}-2\pi i n y\right\}dy+O(x^{3/4}),\ x\to+\infty.$$

Now

$$\int_{-\infty}^{\infty} w^{-3/2}\sum_{n\le x}\exp\left\{\frac{\pi n}{x}-2\pi i n y\right\}dy=\sum_{n\le x} e^{\pi n/x}\int_{-\infty}^{\infty} w^{-3/2}e^{-2\pi i n y}dy,$$

and by [4, p. 35] (again valid for $k=3$),

$$\int_{-\infty}^{\infty} w^{-3/2}e^{-2\pi i n y}dy=\frac{\pi^{3/2}}{\Gamma(3/2)}\,e^{-\pi n/x}n^{1/2}=2\pi e^{-\pi n/x}n^{1/2}.$$

Thus, we have

$$\int_{-\infty}^{\infty} w^{-3/2}\sum_{n\le x}\exp\left\{\frac{\pi n}{x}-2\pi i n y\right\}dy=2\pi\sum_{n\le x} n^{1/2},$$

and (10) becomes

$$A_3(x)=2\pi\sum_{n\le x} n^{1/2}+\sum_{2\le q\le x^{1/2}}\sum_{h(\mathrm{mod}\ q)}{}'\left(\frac{S(h,\,q)}{q}\right)^3$$

$$\int_{\mathfrak{B}(h,\,q)} w^{-3/2}\sum_{n\le x}\exp\left\{\frac{\pi n}{x}-2\pi i n\left(y+\frac{h}{q}\right)\right\}dy+O(x^{3/4}\log x),\ x\to+\infty. \qquad (11)$$

Let Σ denote the multiple sum on the right-hand side of (11); to prove (6) it is sufficient to show that $\Sigma=O(x^{3/4}\log x)$, as $x\to+\infty$.

By (5) and (9),

$$|\Sigma|\le K\sum_{2\le q\le x^{1/2}} q^{-3/2}\sum_{h(\mathrm{mod}\ q)}{}'\int_{|y|\le q^{-1}x^{-1/2}}|w|^{-3/2}\left|\sum_{n\le x}\exp\left\{\frac{\pi n}{x}-2\pi i n\left(y+\frac{h}{q}\right)\right\}\right|dy. \qquad (12)$$

We apply the familiar method of partial summation to estimate the inner sum. Let $T(n)=\sum_{1\le k\le n} e^{-2\pi i k(y+h/q)}$. Then since $T(n)$ is a geometric series

$$|T(n)|\le 2|e^{\pi i(y+h/q)}-e^{-\pi i(y+h/q)}|^{-1}=|\sin\pi\left(y+\frac{h}{q}\right)|^{-1}.$$

Since $|y|\le q^{-1}x^{-1/2}$, $q^{-1}(h-x^{-1/2})\le y+\frac{h}{q}\le q^{-1}(h+x^{-1/2})$, while $q\ge 2$ implies that $1\le h\le q-1$:

thus if $x \geq 1$ (say), $O \leq y + \frac{h}{q} \leq 1$. Therefore

$$|\sin \pi \left(y + \frac{h}{q}\right)|^{-1} \leq \max \left\{\frac{1}{2(y + h/q)}, \frac{1}{2(1 - y - h/q)}\right\}.$$

Also,

$qy + h \geq h - x^{-1/2} \geq h - \frac{1}{2}$, and $q - qy - h \geq q - h - x^{-1/2} \geq q - h - \frac{1}{2}$, if $x \geq 4$. We conclude that

$$|T(n)| \leq q \left\{\frac{1}{2h-1} + \frac{1}{2q-2h-1}\right\} \leq q \left\{\frac{1}{h} + \frac{1}{q-h}\right\}.$$

Now,

$$\sum_{1 \leq n \leq x} \exp \left\{\frac{\pi n}{x} - 2\pi i n \left(y + \frac{h}{q}\right)\right\} = \sum_{1 \leq n \leq x} e^{\pi n/x}\{T(n) - T(n-1)\}$$

$$= \sum_{1 \leq n \leq x} T(n)\{e^{\pi n/x} - e^{\pi(n+1)/x}\} + e^{\pi([x]+1)/x} T([x]),$$

and we have

$$\left|\sum_{1 \leq n \leq x} \exp \left\{\frac{\pi n}{x} - 2\pi i n \left(y + \frac{h}{q}\right)\right\}\right| \leq q \left\{\frac{1}{h} + \frac{1}{q-h}\right\} \sum_{1 \leq n \leq x} \{e^{\pi(n+1)/x} - e^{\pi n/x}\}$$

$$+ q \left\{\frac{1}{h} + \frac{1}{q-h}\right\} e^{\pi([x]+1)/x} \leq 2q \left\{\frac{1}{h} + \frac{1}{q-h}\right\} e^{\pi(x+1)/x} \leq K' q \left\{\frac{1}{h} + \frac{1}{q-h}\right\},$$

where K' is independent of h, q, and x. This, with (12), leads to

$$\Sigma = O\left(\sum_{2 \leq q \leq x^{1/2}} q^{-1/2} \sum_{h \pmod q}{}' \left\{\frac{1}{h} + \frac{1}{q-h}\right\} \int_0^{q^{-1}x^{-1/2}} |w|^{-3/2}\, dy\right), x \to +\infty.$$

But $|w|^{-3/2} = x^{3/2}(1 + 4x^2y^2)^{-3/4} \leq \min\{x^{-3/2}, (2y)^{-3/2}\}$, so that

$$\Sigma = O\left(\sum_{2 \leq q \leq x^{1/2}} q^{-1/2} \sum_{h \pmod q}{}' \left\{\frac{1}{h} + \frac{1}{q-h}\right\} \left\{\int_0^{x^{-1}} x^{3/2}\, dy + \int_{x^{-1}}^{q^{-1}x^{-1/2}} y^{-3/2}\, dy\right\}\right)$$

$$= O\left(\sum_{2 \leq q \leq x^{1/2}} q^{-1/2} \sum_{h \pmod q}{}' \left\{\frac{1}{h} + \frac{1}{q-h}\right\} x^{1/2}\right)$$

$$= O\left(x^{1/2} \sum_{2 \leq q \leq x^{1/2}} q^{-1/2} \log q\right)$$

$$= O(x^{3/4} \log x), \text{ as } x \to +\infty,$$

and (6) is proved.

To obtain (1) we simply apply (7) to $\sum_{1 \leq n \leq x} n^{1/2}$. This gives

$$\sum_{1 \leq n \leq x} n^{1/2} = \int_0^x t^{1/2} dt - \Psi(x) x^{1/2} + \frac{1}{2} \int_0^x \Psi(t) \cdot t^{-1/2} dt = \frac{2}{3} x^{3/2} + O(x^{1/2}), \; x \to +\infty.$$

Together with (6), this implies

$$A_3(x)=\frac{4}{3}\pi x^{3/2}+O(x^{3/4}\log x),\ x\to+\infty,$$

and the proof of (1) is complete.

4. Proof (2)

We begin with two lemmas (cf. [4, pp. 49–50]).

LEMMA 2. $A_k(x)=\sum_{-\sqrt{x}\le m\le\sqrt{x}} A_{k-1}(x-m^2)$, *for* $k\ge 2$.

PROOF: Clear.

LEMMA 3. $\sum_{-\sqrt{x}\le m\le\sqrt{x}} (x-m^2)^{k/2}=\int_{-\sqrt{x}}^{\sqrt{x}}(x-t^2)^{k/2}dt+O(x^{\frac{k-1}{2}}),\ x\to+\infty.$

PROOF: By Lemma 1,

$$\sum_{-\sqrt{x}\le m\le\sqrt{x}}(x-m^2)^{k/2}=\sum_{-\sqrt{x}<m<\sqrt{x}}(x-m^2)^{k/2}=\int_{-\sqrt{x}}^{\sqrt{x}}(x-t^2)^{k/2}dt-k\int_{-\sqrt{x}}^{\sqrt{x}}\Psi(t)(x-t^2)^{\frac{k}{2}-1}tdt.$$

But by the second mean value theorem of the integral calculus,

$$\int_{-\sqrt{x}}^{\sqrt{x}}\Psi(t)(x-t^2)^{\frac{k}{2}-1}tdt=O(x^{\frac{k}{2}-1+\frac{1}{2}})=O(x^{\frac{k-1}{2}}),\ \text{as } x\to+\infty,$$

since $\int_{-\sqrt{x}}^{\sqrt{x}}\Psi(t)dt$ is bounded, independently of x.

To prove (2) we assume

$$R_3(x)=o(x^{1/2}\log\log x),\ x\to+\infty, \tag{13}$$

and show that this leads to a contradiction. By lemma 2, and the definition of $R_3(x)$,

$$A_4(x)=\sum_{-\sqrt{x}\le m\le\sqrt{x}}A_3(x-m^2)=\frac{4}{3}\pi\sum_{-\sqrt{x}\le m\le\sqrt{x}}(x-m^2)^{3/2}+\sum_{-\sqrt{x}\le m\le\sqrt{x}}R_3(x-m^2).$$

By (13), given any $\epsilon>0$ there exists $N>3$ such that if $x>N$, then $|R_3(x)|<\epsilon x^{1/2}\log\log x$. Also (13) implies that for *any* $x>3$, $|R_3(x)|<Kx^{1/2}\log\log x$, where K is independent of x. Therefore, assuming that $x>N$, we have

$$\left|\sum_{-\sqrt{x}\le m\le\sqrt{x}}R_3(x-m^2)\right|\le\sum_{-\sqrt{x-N}<m<\sqrt{x-N}}\left|R_3(x-m^2)\right|+\sum_{\sqrt{x-N}\le|m|\le\sqrt{x}}\left|R_3(x-m^2)\right|$$

$$<2\epsilon(x-N)^{1/2}x^{1/2}\log\log x+\frac{KN}{(x-N)^{1/2}}x^{1/2}\log\log x$$

$$+R_3(0)+R_3(1)+R_3(2),$$

where we have used the fact that $x^{1/2}\log\log x$ is monotone and observed that there are at most $N/(x-N)^{1/2}$ integers in the range $\sqrt{x-N}\leq|m|\leq\sqrt{x}$. Now holding N fixed and letting $x\to+\infty$, we have

$$\overline{\lim_{x\to+\infty}}\ \frac{\left|\sum_{-\sqrt{x}\leq m\leq\sqrt{x}}R_3(x-m^2)\right|}{x\log\log x}\leq 2\epsilon.$$

Since $\epsilon>0$ is arbitrary, we conclude that

$$\sum_{-\sqrt{x}\leq m\leq\sqrt{x}}R_3(x-m^2)=o(x\log\log x),\ \text{as}\ x\to+\infty,$$

so that

$$A_4(x)=\frac{4}{3}\pi\sum_{-\sqrt{x}\leq m\leq\sqrt{x}}(x-m^2)^{3/2}+o(x\log\log x),\ x\to+\infty.$$

Lemma 3, with $k=3$, implies that

$$\sum_{-\sqrt{x}\leq m\leq\sqrt{x}}(x-m^2)^{3/2}=\frac{3}{8}\pi x^2+O(x),\ x\to+\infty,$$

and we get

$$A_4(x)=\frac{\pi x^2}{2}+o(x\log\log x),\ x\to+\infty,$$

in contradiction to (3). Thus (13) is impossible, and the proof of (2) is complete.

5. Remarks

1. The method used here is the derivation of a o-estimate for $R_4(x)$ from an assumed o-estimate for $R_3(x)$. Thus an improved Ω-estimate for $R_4(x)$ would immediately give an improvement on (2), by the same method.

2. This process can be applied to give an O-estimate for $R_3(x)$, given an O-estimate for $R_2(x)$. If we start with Vinogradov's result [2]

$$R_2(x)=O(x^{\frac{17}{53}+\epsilon}),\ \epsilon>0,\ x\to+\infty,$$

we get

$$R_3(x)=O(x^{\frac{87}{106}+\epsilon}),\ \epsilon>0,\ x\to+\infty,$$

an estimate which is, however, weaker than (1).

6. References

[1] K. Chandrasekharan and R. Narashimhan, Hecke's functional equation and the average order of arithmetical functions, Acta Arithmetica **6**, 487–503 (1961).

[2] I. M. Vinogradov, On the number of integral points in the interior of a circle (Russian), Bulletin Acad. Sci. Leningrad **7**, 313–336 (1932).

[3] I. M. Vinogradov, On the number of integral points in a given domain (Russian), Izv Akad. Nauk SSSR Ser. Mat. **24**, 777–786 (1960).

[4] Arnold Walfisz, Gitterpunkte in mehrdimensionalen Kugeln, Warsaw, Panstwowe Wydawnictwo Naukowe (1957).

(Paper 69B4–156)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 69B, No. 4, October–December 1965

Error Analysis of Phase-Integral Methods. I. General Theory for Simple Turning Points

F. W. J. Olver

(July 1, 1965)

An approximate general solution of the differential equation

$$d^2w/dz^2 = f(z)w$$

is

$$w = Af^{-1/4} \exp\left(\int f^{1/2}dz\right) + Bf^{-1/4} \exp\left(-\int f^{1/2}dz\right).$$

To represent a particular solution throughout a given complex domain, differing pairs of values of the arbitrary constants A and B are generally needed in various subdomains. Strict error bounds are established in this paper for the coefficients in the linear equations connecting the pairs of values of A and B, in the case in which the z-domain under consideration is unbounded and contains a simple zero and no singularities of $f(z)$.

The results are used to place the "WKBJ" method on a firm mathematical foundation.

Key Words: Differential equations, asymptotics, phase-integral, WKBJ method, turning point, connection formulas, error bounds.

1. Introduction

A form of solution of the differential equation

$$\frac{d^2w}{dz^2} = f(z)w, \tag{1.01}$$

which is frequently used in applied mathematical problems, is given by

$$w \approx Af^{-1/4} \exp\left(\int f^{1/2}dz\right) + Bf^{-1/4} \exp\left(-\int f^{1/2}dz\right). \tag{1.02}$$

in which A, B are arbitrary constants. This is commonly referred to as the *Liouville-Green approximation*, the *WKB* or *WKBJ approximation*, or the *phase-integral solution*. A necessary condition for the applicability of the approximation is that $f^{-1/4}$ be a bounded, slowly varying function of z [1].[1] This condition automatically excludes from the region of validity most kinds of singularity of f, and also zeros of f, the so-called turning or transition points of the differential equation.

A further condition concerns the monotonicity of the function $\mathrm{Re}\int f^{1/2}dz$ (see [1], sec. 8, and sec. 4, below). This requirement has the effect of dividing the z-region under consideration, **D**, say, into a number of subregions, in each of which a different combination of values of A and B in (1.02) has to be used in order to represent the same solution of (1.01). This is, of course, an example of the Stokes phenomenon. The linear equations linking the values of A and B in one subregion with those in another are called the *connection formulas* or *Stokes equations*. The purpose of this paper is to determine the connection formulas in the case in which **D** contains no singularity of $f(z)$, and just one simple turning point, z_0, say.

[1] Figures in brackets indicate the literature references at the end of this paper.

Two principal methods are available for attacking this problem. The first, applicable when $f(z)$ is real on the real axis, starts with the Liouville-Green approximation in real exponential form on one side of z_0, then traces its behavior along a semicircle in the complex plane to the real axis on the other side of z_0. The condition that the solution must be real when z is real suffices to determine the main features of the appropriate connection formula. This method was originated by Zwaan [2], and has been developed further by Kemble [3] and Furry [4].

The second method consists of using approximations to the solutions in terms of Airy functions (or equivalently Bessel functions of order one-third), the region of validity of which includes z_0. Away from z_0 the Airy functions are approximated by their asymptotic forms for large argument, leading immediately to the Liouville-Green forms. In the original version [5]–[7], the Airy-function representations were constructed by replacing $f(z)$ by a linear approximation in the neighborhood of z_0; this is, perhaps, the true "WKBJ method." In more recent work [8]–[13] more powerful uniform approximations in terms of Airy functions have been used to derive the connection formulas.

Hitherto, the method of Zwaan has not been put on a sound mathematical footing: writing in 1934 Langer [14] commented ". . . an estimation of the relative error involved in the result is almost impossible . . .". The treatment of the Airy-function procedure has been more satisfactory. By supposing that $f(z)$ contains as multiplicative factor (the square of) a large parameter u, say, it is shown in the references cited that the connection formulas are asymptotically correct as $|u| \to \infty$.

In the present paper we give rigorous analytical derivations of both methods, and supply explicit bounds for the errors in the connection formulas (thus overcoming one of Langer's objections to Zwaan's method). Since we are dealing with bounds there is no need for the explicit introduction of a parameter u in the theory: asymptotic properties in applications can be regarded as immediate consequences of the form of error bound.[2] We also dispense with the requirement, in Zwaan's method, that $f(z)$ be real on the axis.

The starting points of our investigation are the theories of error bounds for the Liouville-Green and uniform Airy approximations which have been developed by the writer in [1] and [15].

Since the present paper and its sequel [19] were written, there has appeared a monograph on the same subject by N. Fröman and P. O. Fröman [20]. Although the objective of these authors is essentially the same as that of the present writer, the methods used and results achieved are sufficiently different to warrant publication of this paper and [19] in substantially their original forms. Some comparisons with the results of [20] are given in section 11.

2. First Error Theorem

We begin with the differential equation

$$\frac{d^2w}{dz^2} = \{1 + f(z)\}w, \tag{2.01}$$

in which $f(z)$ is a regular (holomorphic) function in a simply-connected complex z-domain $\mathbf{D}$.

THEOREM 1. *Equation (2.01) has solutions $w_j(z)$ $(j = 1, 2)$ regular in $\mathbf{D}$, and depending on arbitrary fixed points a_j of $\mathbf{D}$, such that*

$$w_j(z) = e^{\pm z}\{1 + \epsilon_j(z)\}, \tag{2.02}$$

where

$$|\epsilon_j(z)|,\ |\epsilon_j'(z)|,\ |\epsilon_j(z) \pm \epsilon_j'(z)| \leqslant \exp\{\mathcal{V}_{\gamma_j}(G)\} - 1 \tag{2.03}$$

when $z \in \mathbf{H}_j$.

[2] In the course of a valuable historical introduction to phase integral methods, Heading ([13], p. 8) critizes other writers, particularly Budden [12], for failing to standardize a large parameter in their analysis. The theory of error bounds presented in this paper provides a broader basis for justifying the work of these writers.

In this result, the upper signs are to be taken when $j=1$, and the lower signs when $j=2$. The regions of validity $\mathbf{H}_j$ $(j=1, 2)$ comprise the aggregate of those points z for which there exists a path $\mathscr{P}_j$ joining z with a_j and lying entirely in $\mathbf{D}$, with the properties:

(i) $\mathscr{P}_j$ consists of a finite number of Jordan arcs, each having a parametric equation of the form $t=t(\tau)$ with $t''(\tau)$ continuous and $t'(\tau)$ nonvanishing.

(ii) Re t is monotonic nonincreasing $(j=1)$ or monotonic nondecreasing $(j=2)$, as t traverses $\mathscr{P}_j$ from z to a_j.

Lastly, $\mathscr{V}_{\mathscr{P}_j}(G)$ denotes the variation along $\mathscr{P}_j$ of the function

$$G(z)=\int f(z)dz; \tag{2.04}$$

thus

$$\mathscr{V}_{\mathscr{P}_j}(G)=\int_z^{a_j}|f(t)dt|. \tag{2.05}$$

Theorem 1 is essentially a special case of Theorem 7 of [1]. We record the main steps of the proof, however, since they are needed in the derivation of further properties of the error terms in the next section.

For illustration, we take $j=1$. From (2.01) and (2.02) we find that

$$\epsilon_1''(z)+2\epsilon_1'(z)=f(z)\{1+\epsilon_1(z)\}. \tag{2.06}$$

Therefore $\epsilon_1(z)$ satisfies the integral equation

$$\epsilon_1(z)=\tfrac{1}{2}\int_{a_1}^{z}\{1-e^{2(t-z)}\}\{1+\epsilon_1(t)\}f(t)dt, \tag{2.07}$$

in which the path of integration is taken to be $\mathscr{P}_1$. The solution of this equation is constructed as a convergent series

$$\epsilon_1(z)=\sum_{n=1}^{\infty}I_{1,n}(z), \tag{2.08}$$

in which $I_{1,0}(z)=1$, and

$$I_{1,n}(z)=\tfrac{1}{2}\int_{a_1}^{z}\{1-e^{2(t-z)}\}f(t)I_{1,n-1}(t)dt \qquad (n\geqslant 1). \tag{2.09}$$

In consequence of Condition (ii) on $\mathscr{P}_1$ we have

$$|e^{2(t-z)}|\leqslant 1, \tag{2.10}$$

and by substituting this bound in (2.09) we readily establish by induction that

$$|I_{1,n}(z)|\leqslant\{\mathscr{V}_{a_1,z}(G)\}^n/n! \qquad (n\geqslant 0), \tag{2.11}$$

showing that the series (2.08) is uniformly convergent. In order that solutions of the integral equation (2.07) also represent solutions of the differential equation (2.06), some restrictions are needed on the path $\mathscr{P}_1$. Those given in (i) above suffice (compare [16], pp. 491–492).

The first of the inequalities (2.03) now follows by summation of (2.11). The other two are derived similarly from the differentiated form of (2.09).

3. Further Properties of the Error Terms

For conciseness, we shall refer to a path $\mathscr{P}_j$ which fulfills Condition (i) of section 2 and is such that Re t is monotonic as t traverses $\mathscr{P}_j$ as a *progressive* path. If the monotonicity is strict everywhere, we say that the path is *strictly progressive*. It may be noted, incidentally, that Condition (i) is quite weak, and can be fulfilled, for example, by any finite chain of straight lines and circular arcs.

The condition that **D** be simply connected, mentioned in the opening paragraph of section 2, merely ensures that each $w_j(z)$ is single-valued in **D**. For a multiply connected domain, each branch of $w_j(z)$ satisfies (2.02) and (2.03) whenever a progressive path can be found in **D** joining z with a_j.

In section 2 we tacitly assumed that the points a_j are finite. Theorem 1 still holds, however, if **D** is unbounded and the a_j are points at infinity on progressive paths $\mathscr{L}_j$, provided that $\mathscr{P}_j$ coincides with $\mathscr{L}_j$ as a_j is approached and that the variations (2.05) converge. The convergence of the infinite integrals (2.09) is then an immediate consequence of the inequality (2.11).

A situation of importance in the later sections occurs when a_1 and a_2 are distinct points at infinity, and can be joined by a progressive path $\mathscr{P}$ lying in **D**. From (2.03) it is seen that $\epsilon_1(z)$ and $\epsilon_1'(z)$ both vanish as $z \to a_1$ along $\mathscr{P}$; indeed we may regard these properties as the boundary conditions defining $w_1(z)$. What happens, however, to $\epsilon_1(z)$ and $\epsilon_1'(z)$ as $z \to a_2$?

THEOREM 2. *If* $|\mathrm{Re}\ z| \to \infty$ *as* $z \to a_1$ *and as* $z \to a_2$, *then*

$$\left.\begin{aligned} &\epsilon_1(z) \to \textit{a constant } \epsilon_1(a_2), \textit{ say, and } \epsilon_1'(z) \to 0 \textit{ as } z \to a_2, \\ &\epsilon_2(z) \to \textit{a constant } \epsilon_2(a_1), \textit{ say, and } \epsilon_2'(z) \to 0 \textit{ as } z \to a_1, \end{aligned}\right\} \tag{3.01}$$

$$\epsilon_1(a_2) = \epsilon_2(a_1), \tag{3.02}$$

and

$$|\epsilon_1(a_2)| \leqslant \tfrac{1}{2}\{\exp\{\mathscr{V}_{\mathscr{P}}(G)\} - 1\}. \tag{3.03}$$

To prove these results, let

$$\alpha_{1,n}(z) = \int_{a_1}^{z} f(t) I_{1,n-1}(t)\,dt, \qquad \beta_{1,n}(z) = \int_{a_1}^{z} e^{2(t-z)} f(t) I_{1,n-1}(t)\,dt. \tag{3.04}$$

Then from (2.08) and (2.09), we have

$$\epsilon_1(z) = \tfrac{1}{2}\Sigma\alpha_{1,n}(z) - \tfrac{1}{2}\Sigma\beta_{1,n}(z), \qquad \epsilon_1'(z) = \Sigma\beta_{1,n}(z), \tag{3.05}$$

the summations extending in each case from $n = 1$ to $n = \infty$. Since by hypothesis $\int_{a_1}^{a_2} |f(t)dt|$ converges, it follows that for any given positive number δ which is less than the value of this doubly infinite integral there exists a point z' on $\mathscr{P}$ such that

$$\int_{z'}^{a_2} |f(t)dt| = \delta. \tag{3.06}$$

Let z be any point of $\mathscr{P}$ between z' and a_2 (fig. 1). Then by splitting the integration range in the second of (3.04) at z', and applying (2.10), (2.11), we find that

$$|\beta_{1,n}(z)| \leqslant |e^{2(z'-z)}| \frac{\{\mathscr{V}_{a_1,z'}(G)\}^n}{n!} + \frac{\{\mathscr{V}_{a_1,a_2}(G)\}^{n-1}}{(n-1)!}\,\delta. \tag{3.07}$$

FIGURE 1.

Therefore

$$|\Sigma\beta_{1,n}(z)| \leq |e^{2(z'-z)}|[\exp\{\mathscr{V}_{a_1,z}(G)\}-1]+\delta\exp\{\mathscr{V}_{a_1,a_2}(G)\}. \tag{3.08}$$

With the assumed conditions, $e^{2(z'-z)}$ vanishes as $z\to a_2$. Hence $\Sigma\beta_{1,n}(z)$ also vanishes, that is, $\epsilon_1'(z)\to 0$.

Next, we have

$$|\alpha_{1,n}(z)-\alpha_{1,n}(z')| = \left|\int_{z'}^{z} f(t)I_{1,n-1}(t)dt\right| \leq \frac{\{\mathscr{V}_{a_1,z}(G)\}^n-\{\mathscr{V}_{a_1,z'}(G)\}^n}{n!}, \tag{3.09}$$

and so

$$|\Sigma\alpha_{1,n}(z)-\Sigma\alpha_{1,n}(z')| \leq \exp\{\mathscr{V}_{a_1,z}(G)\}-\exp\{\mathscr{V}_{a_1,z'}(G)\}. \tag{3.10}$$

The right side of this inequality vanishes as z and z' tend independently to a_2, therefore $\Sigma\alpha_{1,n}(z)$ tends to a constant limiting value. The proof of the first line of (3.01) is now complete. The second line follows by symmetry.

To prove (3.02), we construct the Wronskian from (2.02):

$$\mathscr{W}_{(w_2,w_1)}=\{1+\epsilon_2(z)\}\{1+\epsilon_1(z)+\epsilon_1'(z)\}+\{1+\epsilon_1(z)\}\{1+\epsilon_2(z)-\epsilon_2'(z)\}. \tag{3.11}$$

From (3.01) we see that this reduces to $2\{1+\epsilon_2(a_1)\}$ at $z=a_1$, and $2\{1+\epsilon_1(a_2)\}$ at $z=a_2$. Since the Wronskian is constant, (3.02) follows.

Lastly, we derive from (2.11) and (3.04)

$$|\alpha_{1,n}(a_2)| \leq \{\mathscr{V}_{a_1,a_2}(G)\}^n/n!. \tag{3.12}$$

The improved form (3.03) of the main result (2.03) for the special value $z=a_2$ now follows immediately from (3.05).

4. Basic Error Theorem for the Liouville-Green Approximation

We now proceed to apply the results of the preceding two sections to the differential equation (1.01). A useful generalization is achieved on replacing the coefficient of w in this equation by the sum of two functions $f(z)$ and $h(z)$, say. In applications the second function $h(z)$ will either be zero, or small, in some sense, compared with $f(z)$ (cf. [1], sec. 4(ii)). From the standpoint of the error analysis, however, the relative magnitudes of $f(z)$ and $h(z)$ are immaterial.

Thus we consider the differential equation

$$\frac{d^2w}{dz^2}=\{f(z)+h(z)\}w, \tag{4.01}$$

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in which $f(z)$ and $h(z)$ are regular in an unbounded domain **D**, not necessarily simply connected, and $f(z)$ is nonvanishing. The Liouville transformation

$$\xi = \xi(z) = \int \{f(z)\}^{1/2} dz, \qquad W = \{f(z)\}^{1/4} w, \tag{4.02}$$

throws (4.01) into the form

$$d^2W/d\xi^2 = \{1 + \varphi(\xi)\}W, \tag{4.03}$$

in which

$$\varphi(\xi) = \frac{h(z)}{f(z)} + \frac{4f(z)f''(z) - 5\{f'(z)\}^2}{16\{f(z)\}^3} = \frac{h}{f} - \frac{1}{f^{3/4}} \frac{d^2}{dz^2}\left(\frac{1}{f^{1/4}}\right). \tag{4.04}$$

Equation (4.03) is of the form (2.01). The z-domain **D** is mapped on a ξ-domain **Δ**, say, and $\varphi(\xi)$ is regular in **Δ**. By applying Theorem 1 and then restoring the original variables we establish the following:

THEOREM 3. *Let $z = c$ be an arbitrary point at infinity in* **D** *such that* $|\mathrm{Re}\ \xi(c)| = \infty$, *and let the branch of $\xi(z)$ be chosen in such a way that* $\mathrm{Re}\ \xi(z)$ *is positive as c is approached. Then the differential equation* (4.01) *has a regular solution, given by*

$$w(z) = \{f(z)\}^{-1/4} e^{-\xi(z)} \{1 + \epsilon(z)\}, \tag{4.05}$$

where

$$|\epsilon(z)|,\ |f^{-1/2}\epsilon'(z)|,\ |\epsilon(z) - \{\epsilon'(z)/\xi'(z)\}| \leqslant \exp\{\mathcal{V}_{z,c}(F)\} - 1 \quad (z \in \mathbf{H}(c)), \tag{4.06}$$

and

$$F(z) = \int \varphi(\xi) d\xi = \int \left\{\frac{h}{f^{1/2}} - \frac{1}{f^{1/4}} \frac{d^2}{dz^2}\left(\frac{1}{f^{1/4}}\right)\right\} dz. \tag{4.07}$$

The region of validity $\mathbf{H}(c)$ comprises those points z which can be joined in **D** to c by a "ξ-progressive" path $\mathscr{P}$, that is, one whose map in the ξ-plane is progressive (sec. 3). All branches in (4.05) to (4.07) are continuous along $\mathscr{P}$, that of $f^{1/2}$ being the square of $f^{1/4}$. The variation in (4.06) is taken over $\mathscr{P}$; naturally we assume that it converges at c, otherwise (4.06) is meaningless.

5. Fundamental Connection Formula for a Simple Turning Point

In this section we suppose that $f(z)$ and $h(z)$ are regular in an unbounded, simply connected domain **D**, and that $f(z)$ has just one zero in **D**, a simple zero at an interior point z_0, say. We define $\xi(z)$ by (4.02), fixing the arbitrary lower integration limit at z_0:

$$\xi(z) = \int_{z_0}^{z} \{f(t)\}^{1/2} dt. \tag{5.01}$$

Clearly $\xi(z)$ is an analytic function in **D** whose only singularity is a branch point at z_0. If the Taylor expansion of $f(z)$ in the neighborhood of z_0 is denoted by

$$f(z) = \sum_{n=1}^{\infty} f_n (z - z_0)^n, \tag{5.02}$$

then

$$\xi(z)=\frac{2}{3}f_1^{1/2}(z-z_0)^{3/2}\{1+O(z-z_0)\}. \tag{5.03}$$

The set of points in the z-plane for which

$$\operatorname{Re}\,\xi(z)=0 \tag{5.04}$$

we call the *principal curves* [3] *associated with the turning point* z_0. Using the theory of conformal mapping, we see that each principal curve is a regular Jordan arc which can terminate only at z_0 or at the boundary of **D**. Moreover, no principal curve can intersect itself or any other principal curve except at z_0. Equation (5.03) shows that three principal curves emerge from z_0, inclined there at angle $2\pi/3$ with each other; we denote them by $\mathscr{C}_1, \mathscr{C}_2, \mathscr{C}_3$, enumerated in the positive rotational sense. These and other principal curves divide **D** into a number of subdomains. Those with z_0 on their boundary we call the *principal subdomains*, and denote them by $\mathbf{D}_1$, $\mathbf{D}_2$, $\mathbf{D}_3$, as indicated on figure 2. Clearly each $\mathbf{D}_j$ is itself simply connected. For terminological convenience in what follows we shall enumerate j with modulo 3; thus $\mathbf{D}_0 \equiv \mathbf{D}_3$, $\mathbf{D}_4 \equiv \mathbf{D}_1$.

We define $\xi_j(z)$ $(j=1, 2, 3)$ to be that branch of $\xi(z)$ which is continuous in **D** cut along the corresponding $\mathscr{C}_j$, and whose real part is positive in $\mathbf{D}_j$ and negative in the other two principal subdomains. Analytic continuation across the cut $\mathscr{C}_j$ is expressed by

$$\xi_j\{(z-z_0)e^{\pm 2\pi i}\}=-\xi_j(z-z_0); \tag{5.05}$$

compare (5.03). We define $g(z)$ to be the four-valued function

$$g(z)=\{f(z)\}^{-1/4}. \tag{5.06}$$

Its analytic continuation is expressed by

$$g\{(z-z_0)e^{\pm 2\pi i}\}=\mp ig(z-z_0). \tag{5.07}$$

We denote by $g_j(z)$ $(j=1, 2, 3)$ an arbitrary constant multiple of any branch of $g(z)$ which is continuous in **D** cut along the corresponding $\mathscr{C}_j$. In order to achieve a symmetric form of final result, we stipulate that these multiples must be chosen in such a way that

$$g_j(z)=e^{\pi i/6}g_{j-1}(z) \qquad (z\in \mathbf{D}_{j-1}\cup \mathbf{D}_j). \tag{5.08}$$

[3] Also called anti-Stokes lines [12], [13].

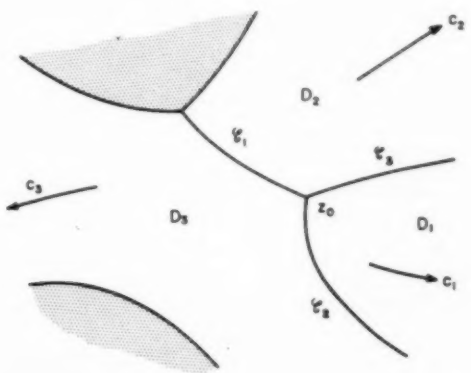

FIGURE 2. *Principal subdomains* $\mathbf{D}_j$.

The self-consistency of this equation for $j=1, 2, 3$ follows from (5.07).

Let us suppose that each $\mathbf{D}_j$ is unbounded, and that c_j is an arbitrary point at infinity in $\mathbf{D}_j$ such that $|\mathrm{Re}\ \xi(c_j)|=\infty$. Excluding the point z_0 from $\mathbf{D}$, and then applying Theorem 3 of section 4, we find that eq (4.01) has solutions $w_j(z)$ $(j=1, 2, 3)$, given by

$$w_j(z)=g_j(z)e^{-\xi_j(z)}\{1+\epsilon_j(z)\}, \tag{5.09}$$

where

$$|\epsilon_j(z)|, |f^{-1/2}\epsilon_j'(z)|, |\epsilon_j(z)-f^{-1/2}\epsilon_j'(z)| \leqslant \exp\{\mathscr{V}_{z, c_j}(F)\}-1 \qquad (z\in \mathbf{H}(c_j)) \tag{5.10}$$

and F is defined by (4.07). In (5.10) the branch of $f^{-1/2}$ is $1/\xi_j'(z)$, and $\mathbf{H}(c_j)$ is the set of z-points which can be joined to c_j by a ξ-progressive path $\mathscr{P}_j$ lying in $\mathbf{D}$. (We observe, in passing, that the corresponding principal curve $\mathscr{C}_j$ is excluded from $\mathbf{H}(c_j)$, since passage of $\mathscr{P}_j$ through z_0 is not permitted.) $\mathscr{V}_{z, c_j}(F)$ denotes the variation over $\mathscr{P}_j$ of F.

Although each solution $w_j(z)$ satisfies (5.09) and (5.10) in only part of $\mathbf{D}$, the theory of linear differential equations shows that each $w_j(z)$ exists and is regular throughout the whole of $\mathbf{D}$. Further, there is an identity of the form

$$A_1w_1(z)+A_2w_2(z)+A_3w_3(z)=0, \tag{5.11}$$

in which the A_j are independent of z. Equation (5.11) is the connection formula for the turning point z_0, and the values of the A_j constitute our primary quest. In order to obtain them, we assume that ξ-progressive paths exist in $\mathbf{D}$ linking each pair of reference points c_j, c_k.

Consider (5.11) in $\mathbf{D}_1$. Substituting by means of (5.09) and (5.08), and using the relations $\xi_2(z)=\xi_3(z)=-\xi_1(z)$, we derive

$$A_1e^{-\xi_1(z)}\{1+\epsilon_1(z)\}+A_2e^{(\pi i/6)+\xi_1(z)}\{1+\epsilon_2(z)\}+A_3e^{-(\pi i/6)+\xi_1(z)}\{1+\epsilon_3(z)\}=0. \tag{5.12}$$

Now let $z\to c_1$. Then $\epsilon_1(z)$ vanishes and, by Theorem 2, $\epsilon_2(z)$ and $\epsilon_3(z)$ tend to constant values $\epsilon_2(c_1)$ and $\epsilon_3(c_1)$. Also by hypothesis $\mathrm{Re}\ \xi_1(z)\to+\infty$. Hence we have

$$e^{\pi i/6}\{1+\epsilon_2(c_1)\}A_2+e^{-\pi i/6}\{1+\epsilon_3(c_1)\}A_3=0. \tag{5.13}$$

Similarly,

$$e^{-\pi i/6}\{1+\epsilon_1(c_2)\}A_1+e^{\pi i/6}\{1+\epsilon_3(c_2)\}A_3=0, \tag{5.14}$$

$$e^{\pi i/6}\{1+\epsilon_1(c_3)\}A_1+e^{-\pi i/6}\{1+\epsilon_2(c_3)\}A_2=0. \tag{5.15}$$

The consistency of this set of homogeneous equations for the A_j immediately follows from the relation $\epsilon_j(c_k)=\epsilon_k(c_j)$ obtained from eq (3.02). Solving for the A_j and substituting back in (5.11), we arrive at the desired form of the connection formula:

$$\{1+\epsilon_2(c_3)\}w_1(z)+e^{-2\pi i/3}\{1+\epsilon_3(c_1)\}w_2(z)+e^{2\pi i/3}\{1+\epsilon_1(c_2)\}w_3(z)=0. \tag{5.16}$$

The error terms are bounded by (compare (3.03))

$$|\epsilon_j(c_k)| \leqslant \tfrac{1}{2}[\exp\{\mathcal{V}_{c_j,c_k}(F)\}-1],$$

that is,

$$|\epsilon_j(c_k)| \leqslant \frac{1}{2}\exp\left\{\int_{c_j}^{c_k}\left|\frac{h}{f^{1/2}}-\frac{1}{f^{1/4}}\frac{d^2}{dz^2}\left(\frac{1}{f^{1/4}}\right)\right||dz|\right\}-\frac{1}{2}. \tag{5.17}$$

in which the variation (or integral) is evaluated along a ξ-progressive path linking c_j with c_k.

We summarize this section so far. The assumed conditions on $f(z)$ and $h(z)$ are stated in the opening sentence. The principal subdomains $\mathbf{D}_j$ associated with the turning point z_0 are defined in the second paragraph. Three solutions $w_j(z)$ $(j=1, 2, 3)$ of the differential equation (4.01) are then constructed, given by (5.09) and (5.10). Here $\xi_j(z)$ is the branch of the integral (5.01) which has positive real part in $\mathbf{D}_j$; $g_j(z)$ $(j=1, 2, 3)$ is any set of constant multiples of branches of $\{f(z)\}^{-1/4}$ satisfying (5.08); c_j is any point at infinity in $\mathbf{D}_j$ such that $|\mathrm{Re}\ \xi(c_j)|=\infty$. The error bounds (5.10) are valid at all points z which can be joined to c_j by a ξ-progressive path lying in $\mathbf{D}$. Finally, provided that the c_j can be joined in pairs by paths of this kind, the fundamental connection formula between the $w_j(z)$ is expressed by (5.16) and (5.17).

Remark. It will be observed that an outstanding problem in the application of the connection formula (5.16) will be the determination of suitable ξ-progressive paths linking together the points at infinity c_j. This appears to be an unavoidable feature of this method,[4] and its solution will generally necessitate a study of the actual conformal transformation between the ξ and z-planes.

Usually it will not be difficult to demonstrate the existence of suitable ξ-progressive paths. These paths are not unique, however, and the most effective use of the connection formula clearly calls for the determination of those paths which minimize the total variation of the function F along their length. Roughly speaking, this means that we need to keep the ξ-progressive paths as far away as possible from all the singularities of $f(z)$ and $h(z)$ and zeros of $f(z)$ (including z_0), subject to fulfillment of the monotonicity condition.

The construction of ξ-progressive paths in the neighborhood of infinity is discussed in section 7 below, and an example of the determination of ξ-progressive paths which minimize the variation of an analytic function along their length is given in [17], section 7.

6. Airy's Equation

The simplest example to which the theory of section 5 is applicable is provided by the differential equation

$$d^2w/dz^2 = zw. \tag{6.01}$$

In the notation of sections 4 and 5, we take $f(z)=z$ and $h(z)=0$. Then $z_0=0$ and

$$\xi(z)=\frac{2}{3}z^{3/2}, \qquad g(z)=z^{-1/4}. \tag{6.02}$$

$\mathbf{D}$ comprises the whole z-plane, and the principal subdomains $\mathbf{D}_j$ are the sectors of angle $2\pi/3$ indicated in figure 3.

We define $g_1(z)$ to be the principal branch of $z^{-1/4}$. Then from (5.08)

$$g_2(z)=e^{\pi i/6}z^{-1/4} \quad (z\in\mathbf{D}_1\cup\mathbf{D}_2), \qquad g_3(z)=e^{-\pi i/6}z^{-1/4} \quad (z\in\mathbf{D}_1\cup\mathbf{D}_3). \tag{6.03}$$

[4] Compare [20], chapter 4.

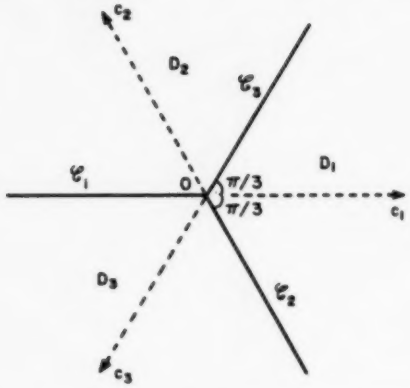

FIGURE 3. *Principal subdomains for Airy's equation.*

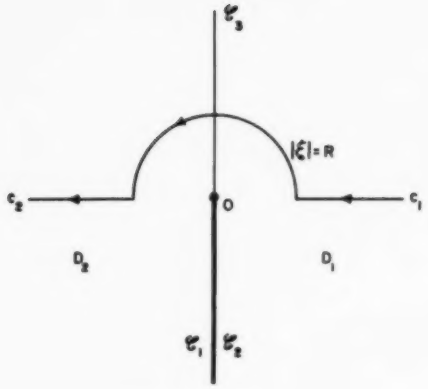

FIGURE 4. *ξ-plane.*

We take $c_1 = +\infty$, $c_2 = \infty e^{2\pi i/3}$, $c_3 = \infty e^{-2\pi i/3}$. By considering the ξ-map we see that each region $\mathbf{H}(c_j)$ comprises the part of the z-plane remaining after the removal of the corresponding principal curve $\mathscr{C}_j$. From (4.07) we have

$$F(z) = \frac{5}{24z^{3/2}} = \frac{5}{36\xi}. \tag{6.04}$$

The ξ-map of a suitable ξ-progressive path linking c_1 with c_2 is shown in figure 4. As the radius R of the semicircular part tends to infinity, the variation of F along the whole path vanishes. Therefore from (5.17) $\epsilon_1(c_2) = 0$. Similarly $\epsilon_2(c_3)$ and $\epsilon_3(c_1)$ both vanish. Accordingly (5.16) reduces to

$$w_1(z) + e^{-2\pi i/3} w_2(z) + e^{2\pi i/3} w_3(z) = 0. \tag{6.05}$$

By comparing (5.09) with the asymptotic forms of the Airy functions [18], we identify

$$w_1(z) = 2\pi^{1/2}\,\mathrm{Ai}\,(z), \quad w_2(z) = 2\pi^{1/2}\,\mathrm{Ai}\,(ze^{-2\pi i/3}), \qquad w_3(z) = 2\pi^{1/2}\,\mathrm{Ai}\,(ze^{2\pi i/3}). \tag{6.06}$$

Equation (6.05) is the well-known connection formula for these functions. It is interesting to observe that our theory yields it *exactly*.

The vanishing of the error terms in this example is essentially a consequence of there being no boundary of $\mathbf{D}$ intervening between c_j and c_k in the neighborhood of infinity. The path of figure 4 generally cannot be used to establish this in other cases. Using different paths, we formulate sufficient conditions for the vanishing of $\epsilon_j(c_k)$ in the next section.

7. Sufficient Conditions for the Vanishing of the Error Terms

We again use the notation of section 5, and we suppose, without loss of generality, that the turning point z_0 is at the origin.

THEOREM 4. *Let $f(z)$ and $h(z)$ be regular in the sector* $\mathbf{S}$: $\gamma_1 < \arg z < \gamma_2$ *for all sufficiently large $|z|$, and*

$$f(z) \sim Az^r, \qquad h(z) = O(z^{(r/2)-1-\delta}), \text{ as } |z| \to \infty, \tag{7.01}$$

uniformly with respect to $\arg z$ *in* $\mathbf{S}$. *Here A is a real or complex non-zero constant, and r, δ real*

constants such that[5] $r > -2$, $\delta > 0$. *Also, within* $\mathbf{S}$, *let* $\mathscr{L}_1$, $\mathscr{L}_2$ *be outward-drawn rays from the origin which lie in adjacent principal subdomains* $\mathbf{D}_1$, $\mathbf{D}_2$, *respectively. Then provided that* $\mathscr{L}_1$, $\mathscr{L}_2$ *are not parallel to the asymptotes of the neighboring boundaries of* $\mathbf{D}_1$, $\mathbf{D}_2$, *they are strictly* ξ*-progressive paths in the neighborhood of infinity, and if* c_1, c_2 *denote the points at infinity on them,* $\epsilon_1(c_2) = 0$.

To prove this result, we first observe that

$$g(z) \equiv \{f(z)\}^{-1/4} \sim A^{-1/4} z^{-r/4} \tag{7.02}$$

as $|z| \to \infty$ in $\mathbf{S}$. Hence ([10], section 1.36)

$$g''(z) \sim \frac{r}{4}\left(\frac{r}{4}+1\right) A^{-1/4} z^{-(r/4)-2} \quad (r \neq 0) \tag{7.03}$$

as $|z| \to \infty$ in any sector $\mathbf{S}' : \gamma_1' < \arg z < \gamma_2'$ which is properly interior to $\mathbf{S}$. When $r = 0$, the result corresponding to (7.03) is $g''(z) = o(z^{-2})$. Therefore, whether or not r is zero, we have

$$g(z)g''(z) = O(z^{-s-1}) \tag{7.04}$$

as $|z| \to \infty$ in $\mathbf{S}'$, uniformly with respect to $\arg z$, where

$$s = \tfrac{1}{2}r + 1,$$

and is positive, by hypothesis. From (4.07), (7.01), and (7.04) we derive

$$F'(z) = O(z^{-1-\delta_1}), \tag{7.05}$$

where $\delta_1 = \min(\delta, s)$. Hence the integral in (5.17) converges. The essential problem is to show how to construct a ξ-progressive path connecting c_1 with c_2 in the neighborhood of infinity.

From (5.01), we have

$$\xi = \frac{A^{1/2} z^s}{s} + o(z^s) \qquad (z \in \mathbf{S}). \tag{7.06}$$

Therefore the principal curves approach infinity in directions parallel to the rays

$$\arg z = \{(n + \tfrac{1}{2})\pi - \tfrac{1}{2}\alpha\}/s, \tag{7.07}$$

where $\alpha = \arg A$, and $n = 0, \pm 1, \pm 2, \ldots$. We call these the *principal directions*. Consider the behavior of $\operatorname{Re} \xi$ along the ray with parametric equation $z = \tau e^{i\gamma}$, γ being real and fixed, and $0 < \tau < \infty$. We have

$$d\xi/d\tau = \{f(z)\}^{1/2}(dz/d\tau) = A^{1/2}\tau^{r/2}e^{is\gamma}\{1 + o(1)\} \tag{7.08}$$

as $\tau \to \infty$. Hence

$$d\,(\operatorname{Re} \xi)/d\tau = |A|^{1/2}\tau^{r/2}\{\cos\,(s\gamma + \tfrac{1}{2}\alpha) + o(1)\}. \tag{7.09}$$

The constant $\cos\,(s\gamma + \frac{1}{2}\alpha)$ vanishes only when γ has one of the values given by the right of (7.07). *Therefore any outward ray in* $\mathbf{S}$ *not in a principal direction is a strictly* ξ*-progressive path for all sufficiently large* $|z|$. In particular this includes $\mathscr{L}_1$ and $\mathscr{L}_2$.

[5] Thus the differential equation (4.01) has an irregular singularity at infinity.

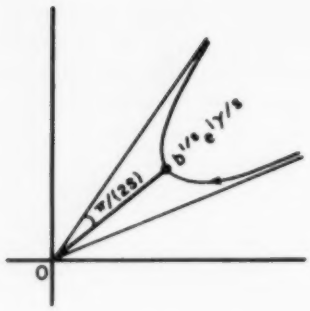

FIGURE 5. *z-plane.*

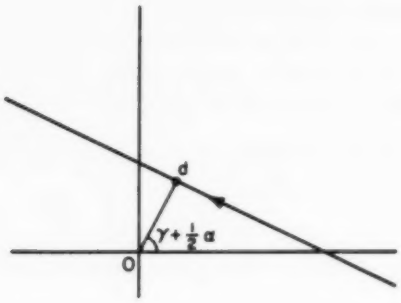

FIGURE 6. *Approximate path in ξ-plane: $|d|=|A|^{1/2}b/s$.*

Next, consider the path with parametric equation

$$z=\{(b+i\tau)e^{i\gamma}\}^{1/s} \qquad (-\infty<\tau<\infty), \tag{7.10}$$

where γ and b are real constants, b being large and positive.

As indicated in figure 5 this path begins at infinity, sweeps back to its nearest approach to the origin at $z=b^{1/s}e^{i\gamma/s}$ and then returns to infinity, the angle between its asymptotes being π/s. When b is large, we have from (7.06)

$$\xi \sim s^{-1}|A|^{1/2}(b+i\tau)e^{i\{\gamma-(\alpha/2)\}},$$

showing that the ξ-map of (7.10) is approximately the straight line indicated in figure 6. Corresponding to (7.09), we find that

$$\frac{d}{d\tau}(\operatorname{Re}\xi)=-\frac{|A|^{1/2}}{s}\left\{\sin\left(\gamma+\frac{1}{2}\alpha\right)+o(1)\right\}, \tag{7.11}$$

as $b\to\infty$, uniformly with respect to τ. Therefore *the curve (7.10) is a strictly ξ-progressive path for all sufficiently large b, except when its asymptotes are in principal directions.*

Now consider c_1 and c_2. By taking γ_1' and γ_2' sufficiently close to γ_1 and γ_2, respectively, we can ensure that $\mathbf{S}'$ contains $\mathscr{L}_1$ and $\mathscr{L}_2$. From (7.06) and the hypotheses on $\mathscr{L}_1$ and $\mathscr{L}_2$, it follows that

$$|\arg c_2-\arg c_1|<2\pi/s. \tag{7.12}$$

Figure 7 indicates how c_1 and c_2 can be connected by a strictly ξ-progressive path in $\mathbf{S}'$, consisting of $\mathscr{L}_1$, $\mathscr{L}_2$ and either one or two arcs of the type (7.10), depending whether or not $|\arg c_2-\arg c_1|<\pi/s$. The corresponding path in the ξ-plane is approximately that indicated in figure 8. On letting the b-parameters of the arcs tend to infinity, we see immediately from (7.05) that the variations of F along $\mathscr{L}_1$ and $\mathscr{L}_2$ tend to zero. For the contribution to the variation from the arcs (7.10), we observe that the corresponding values of $\int|z^{-1-\delta_1}dz|$ are bounded by

$$\frac{1}{s}\int_{-\infty}^{\infty}\frac{d\tau}{|b+i\tau|^{1+(\delta_1/s)}}$$

and accordingly vanish as $b\to\infty$. The proof of Theorem 4 is now complete.

An alternative set of sufficient conditions for the vanishing of the error terms is provided by the next theorem, which can be proved in a similar way. In this result m, A denote real or complex nonzero constants, and δ is a positive constant.

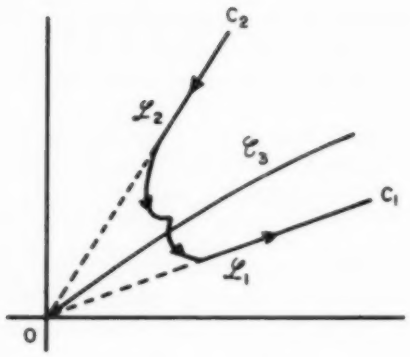

FIGURE 7. *ξ-progressive path in z-plane.*

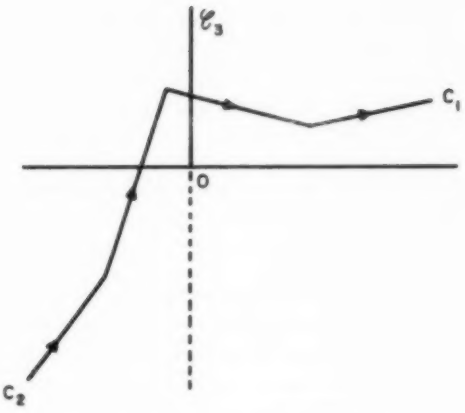

FIGURE 8. *Approximate path in ξ-plane.*

THEOREM 5. *Let $f(z)$ and $h(z)$ be regular in the strip* **T:** $\gamma_1 < \mathrm{Im}(mz) < \gamma_2$ *for all sufficiently large positive values of* Re (mz), *and*

$$f(z) \sim Ae^{mz}, \qquad h(z) = O(e^{mz(1-\delta)2}), \text{ as } \mathrm{Re}\ (mz) \to +\infty, \tag{7.13}$$

uniformly with respect to Im (mz) *in* **T**. *Also, within* **T**, *let* $\mathscr{L}_1$, $\mathscr{L}_2$ *be straight lines which are parallel to the boundaries of* **T**, *and lie in adjacent principal subdomains* $\mathbf{D}_1$, $\mathbf{D}_2$, *respectively. Then provided that* $\mathscr{L}_1$, $\mathscr{L}_2$ *do not coincide with the asymptotes of the boundaries of* $\mathbf{D}_1$, $\mathbf{D}_2$, *they are strictly ξ-progressive paths in the neighborhood of infinity, and if* c_1, c_2 *are the points at infinity on them,* $\epsilon_1(c_2) = 0$.

8. The Gans-Jeffreys Connection Formulas (i)

The first of these two formulas may be regarded as a special case of the fundamental connection formula of section 5. We again consider the differential equation (4.01) in which $f(z)$ and $h(z)$ are regular in an unbounded, simply connected domain **D** and $f(z)$ has just one zero in **D**, a simple zero at $z=0$. This time we suppose that **D** includes the whole of the real axis, and that $f(z)$ and $h(z)$ are real when z is real. Without loss of generality, we take $f(z)/z$ to be positive on the real axis.

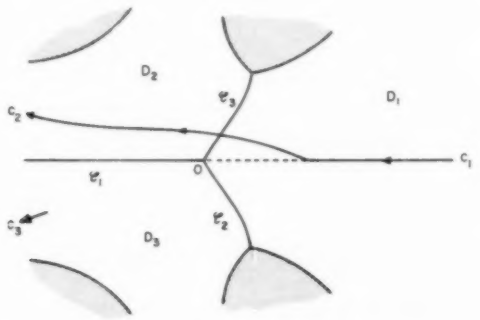

FIGURE 9. *Typical principal subdomains* $\mathbf{D}_j$ *for the Gans-Jeffreys formulas.*

One of the three principal curves, say $\mathscr{C}_1$, which emerges from the origin is the negative real axis. The other two emerge at directions $\pm\pi/3$ and are symmetric with respect to the real axis. As in section 5 we denote by $\mathbf{D}_1$, $\mathbf{D}_2$, $\mathbf{D}_3$ the three subdomains bounded by the principal curves which have the origin on their boundary.

We take c_1 to be the point at infinity on the positive real axis, and c_2, c_3 to be points at infinity on conjugate ξ-progressive curves $\mathscr{L}_2$, $\mathscr{L}_3$. These curves must lie within $\mathbf{D}_2$, $\mathbf{D}_3$, respectively, and be such that no boundary of $\mathbf{D}$ intervenes between them in the neighborhood of infinity. We assume that $|\mathrm{Re}\ \xi(z)| \to \infty$ when $z \to c_j$ $(j=1, 2, 3)$ (the "dominancy condition") and that the variation of the function F, defined by (4.07), converges when $z \to c_j$. The other assumptions we need are

(i) ξ-progressive paths can be found in $\mathbf{D}$ which link c_2 or c_3 with any point of the real axis, other than the origin, and which do not pass through the origin.

(ii) $\epsilon_2(c_3)$, $\epsilon_2(-\infty)$ and $\epsilon_3(-\infty)$ all vanish.

In applications, Condition (i) can be tested by considering the ξ-map. Sufficient sets of conditions for (ii) are to be found in section 7.

The connection formula (5.16) for the solutions of (4.01) takes the form

$$w_1(z) = e^{\pi i/3}\{1+\epsilon_3(c_1)\}w_2(z) + e^{-\pi i/3}\{1+\epsilon_2(c_1)\}w_3(z). \tag{8.01}$$

To fix the solutions completely, we define $g_1(z)$ to be the branch of $\{f(z)\}^{-1/4}$ which takes its principal value on the positive real axis (compare (5.08)). The branches of the $w_j(z)$ are then interpreted in real form as follows.

When z is positive, we have immediately from (5.09) and (5.10)

$$w_1(z) = f^{-1/4} \exp\left(-\int_0^z f^{1/2}dz\right)\{1+\epsilon_1(z)\} \qquad (z>0), \tag{8.02}$$

where

$$|\epsilon_1(z)| \leqslant \exp\{V_{z,\infty}(F)\} - 1, \tag{8.03}$$

the variation being taken along the real axis.

When z is negative, we find that

$$\xi_2(z) = i\int_z^0 |f|^{1/2}dz, \qquad g_2(z) = e^{-\pi i/12}|f|^{-1/4}. \tag{8.04}$$

Substitution of (5.09) in (8.01) accordingly yields

$$w_1(z) = \{1+\epsilon_3(c_1)\}e^{\pi i/4}|f|^{-1/4} \exp\left(-i\int_z^0 |f|^{1/2}dz\right)\{1+\epsilon_2(z)\} + \text{conjugate}. \tag{8.05}$$

Let

$$1+\epsilon_2(z) = \{1+\mu(z)\}e^{-i\eta(z)}, \qquad 1+\epsilon_3(z) = \{1+\mu(z)\}e^{i\eta(z)}, \tag{8.06}$$

where $\mu(z)$ and $\eta(z)$ are real and $\mu(z) \geqslant -1$. Then by elementary considerations

$$|\mu(z)| \leqslant |\epsilon_2(z)|, \qquad |\eta(z)| \leqslant \sin^{-1}|\epsilon_2(z)| \leqslant \pi|\epsilon_2(z)|/2, \tag{8.07}$$

provided that $|\epsilon_2(z)| \leqslant 1$. Substitution in (8.05) yields

$$w_1(z) = 2\{1+\mu(c_1)\}\{1+\mu(z)\}|f|^{-1/4} \sin\left\{\int_z^0 |f|^{1/2}dz + \frac{1}{4}\pi + \eta(z) - \eta(c_1)\right\} \qquad (z<0). \tag{8.08}$$

From (8.07), (5.17) and (5.10), we deduce that

$$|\mu(c_1)|,\ |2\eta(c_1)/\pi| \leqslant \frac{1}{2}\left[\exp\left\{\mathcal{V}_{c_1,c_2}(F)\right\}-1\right], \tag{8.09}$$

and

$$|\mu(z)|,\ |2\eta(z)/\pi| \leqslant \exp\left\{\mathcal{V}_{z,c_2}(F)\right\}-1, \tag{8.10}$$

the variations in both cases being evaluated along ξ-progressive curves.

The aggregate of (8.02), (8.03), (8.08), (8.09), and (8.10), may be regarded as the full form of the first Gans-Jeffreys connection formula [5], [6], [9]. It expresses the subdominant exponential solution on one side of the turning point in terms of the oscillatory solutions on the other side. Boundary conditions satisfied by $w_1(z)$ are clearly

$$\epsilon_1(z)=o(1) \qquad (z\to+\infty); \qquad \mu(z),\ \eta(z)=o(1) \qquad (z\to-\infty). \tag{8.11}$$

We note that the bounds for the error terms $\mu(c_1)$, $\eta(c_1)$ depend solely on the variation of F along the ξ-progressive path linking c_1 and c_2, and can be minimized by proper choice of path.

The second connection formula concerns the dominant exponential solution. Unlike the subdominant solution, this is not unique. Consider first $w_2(z)$. For negative z, we have from (8.04) and (5.09)

$$w_2(z)=e^{-\pi i/12}|f|^{-1/4}\exp\left(-i\int_z^0|f|^{1/2}dz\right)\{1+\epsilon_2(z)\} \qquad (z<0). \tag{8.12}$$

On the other side of the turning point

$$w_2(z)=e^{\pi i/6}f^{-1/4}\exp\left(\int_0^z f^{1/2}dz\right)\{1+\epsilon_2(z)\} \qquad (z>0). \tag{8.13}$$

Instead of $w_2(z)$, however, we prefer the real solution $w_4(z)=\mathrm{Re}\{e^{-\pi i/6}w_2(z)\}$. Then with the aid of (8.06), we derive

$$w_4(z)=[1+\mathrm{Re}\{\epsilon_2(z)\}]f^{-1/4}\exp\left(\int_0^z f^{1/2}dz\right) \qquad (z>0), \tag{8.14}$$

and

$$w_4(z)=\{1+\mu(z)\}|f|^{-1/4}\cos\left\{\int_z^0|f|^{1/2}dz+\frac{1}{4}\pi+\eta(z)\right\} \qquad (z<0), \tag{8.15}$$

where $|\epsilon_2(z)|$, $|\mu(z)|$ and $|2\eta(z)/\pi|$ are all bounded by the right of (8.10). These relations constitute the second Gans-Jeffreys formula. We note that $w_4(z)$ satisfies the boundary conditions

$$\epsilon_2(z)=\epsilon_2(c_1)+o(1) \qquad (z\to+\infty); \qquad \mu(z),\ \eta(z)=o(1) \qquad (z\to-\infty); \tag{8.16}$$

where $|\epsilon_2(c_1)|$ is bounded by the right of (8.09).

9. The Gans-Jeffreys Connection Formulas (ii)

In this section we attack the problem of section 8 with real-variable theory. Our hypotheses are

(i) The function $f(z)/z$ is positive and twice-continuously differentiable throughout the interval $-\infty<z<\infty$, and $h(z)$ is a continuous real function in the same interval.

(ii) As $z \to \pm\infty$, $\left|\int_0^z f^{1/2}dz\right|$ is unbounded and the variation of the function F (defined by (4.07)) converges.

In these circumstances it is shown in [15], sections 4, 5 that (4.01) has a solution [6]

$$w_1(z) = (\zeta/f)^{1/4}\{\mathrm{Ai}\,(\zeta) + \epsilon_1(z)\}, \tag{9.01}$$

where

$$\zeta \equiv \zeta(z) = \pm\left|\frac{3}{2}\int_0^z \{f(t)\}^{1/2}dt\right|^{2/3} \tag{9.02}$$

$$|\epsilon_1(z)| \leqslant \lambda_1^{-1}E^{-1}(\zeta)M(\zeta)[\exp\{\lambda_1 \mathcal{V}_{z,\infty}(H)\} - 1] \quad (-\infty < z < \infty), \tag{9.03}$$

and

$$H(z) = \frac{5}{24|\zeta|^{3/2}} \pm \int^z \left\{\frac{1}{|f|^{1/4}}\frac{d^2}{dz^2}\left(\frac{1}{|f|^{1/4}}\right) - \frac{h}{|f|^{1/2}}\right\}dz. \tag{9.04}$$

The upper or lower signs are taken in (9.02) and (9.04) according as z is positive or negative, and the integration limits in (9.04) are determined by the condition $H(0) = 0$. The auxiliary functions $E(\zeta)$, $M(\zeta)$ and the constant $\lambda_1 = 1.430\ \ldots$ are defined in [15], section 2.

On substituting for Ai (ζ) by means of its appropriate asymptotic forms, we obtain

$$w_1(z) = \tfrac{1}{2}\pi^{-1/2}f^{-1/4}\{1 + o(1)\}\exp\left(-\int_0^z f^{1/2}dz\right) \qquad (z \to +\infty), \tag{9.05}$$

and

$$w_1(z) = \pi^{-1/2}|f|^{-1/4}\left[\sin\left(\int_z^0 |f|^{1/2}dz + \frac{1}{4}\pi\right) + \rho(z) + o(1)\right] \qquad (z \to -\infty), \tag{9.06}$$

where

$$\rho(z) = \pi^{1/2}|\zeta|^{1/4}\epsilon_1(z), \tag{9.07}$$

and is bounded.

In order to throw (9.06) fully into "modulus-phase" form, we appeal to Theorem 4 of [1]. This shows that solutions of (4.01) exist of the form

$$|f|^{-1/4}\{1 + o(1)\}\exp\left\{\pm i\int_z^0 |f|^{1/2}dz\right\} \text{ as } z \to -\infty. \tag{9.08}$$

Therefore we can express

$$w_1(z) = \pi^{-1/2}|f|^{-1/4}\{1 + \nu_1 + o(1)\}\sin\left\{\int_z^0 |f|^{1/2}dz + \frac{1}{4}\pi + \nu_2 + o(1)\right\} \qquad (z \to -\infty), \tag{9.09}$$

where ν_1, ν_2 are real constants to be determined. Comparison of (9.06) with (9.09) shows that

$$\rho(z) = (1 + \nu_1)\sin\{\theta(z) + \nu_2\} - \sin\theta(z) + o(1), \tag{9.10}$$

[6] Not to be confused with the $w_1(z)$ of section 8.

where

$$\theta(z) \equiv \int_z^0 |f|^{1/2} dz + \frac{1}{4}\pi. \tag{9.11}$$

Hence $\rho(z)$ has the form

$$\rho(z) = \rho_L \sin\{\theta(z) + \nu_3\} + o(1), \tag{9.12}$$

where ρ_L and ν_3 are real constants ($\rho_L \geqslant 0$) related to ν_1 and ν_2. Clearly

$$\rho_L = \overline{\lim_{z \to -\infty}} |\rho(z)|. \tag{9.13}$$

Accordingly, from (9.03), (9.07) and the fact that $|\zeta|^{1/4} M(\zeta) \to \pi^{-1/2}$ as $\zeta \to -\infty$, we have

$$\rho_L \leqslant \lambda_1^{-1} [\exp\{\lambda_1 \mathscr{V}_{-\infty, z}(H)\} - 1]. \tag{9.14}$$

In (9.10) and (9.12) let $z \to -\infty$ through a sequence of values for which $\theta(z)$ is an integral multiple of π (compare hypothesis (ii) above). This gives

$$(1 + \nu_1) \sin \nu_2 = \rho_L \sin \nu_3. \tag{9.15}$$

Alternatively, by using a sequence of odd integral multiples of $\frac{1}{2}\pi$ we derive

$$(1 + \nu_1) \cos \nu_2 - 1 = \rho_L \cos \nu_3. \tag{9.16}$$

Combination of (9.15) and (9.16) yields

$$(1 + \nu_1) e^{i\nu_2} = 1 + \rho_L e^{i\nu_3}. \tag{9.17}$$

Therefore

$$|\nu_1| \leqslant \rho_L, \qquad |\nu_2| \leqslant \sin^{-1}\rho_L \leqslant \pi\rho_L/2, \tag{9.18}$$

provided that $\rho_L \leqslant 1$ (compare (8.07)).

The first Gans-Jeffreys formula is represented by the aggregate of (9.05), (9.09), (9.14), and (9.18).

A second solution of (4.01) is [15]

$$w_2(z) = (\zeta/f)^{1/4} \{\mathrm{Bi}(\zeta) + \epsilon_2(z)\}, \tag{9.19}$$

where

$$|\epsilon_2(z)| \leqslant (\lambda_2/\lambda_1) E(\zeta) M(\zeta) [\exp\{\lambda_1 \mathscr{V}_{-\infty, z}(H)\} - 1], \tag{9.20}$$

and $\lambda_2 = 1.315\ldots$. Substitution of the asymptotic forms for $\mathrm{Bi}(\zeta)$ yields

$$w_2(z) = \pi^{-1/2} f^{-1/4} \{1 + \sigma(z) + o(1)\} \exp\left(\frac{2}{3}\zeta^{3/2}\right) \qquad (z \to +\infty), \tag{9.21}$$

and

$$w_2(z) = \pi^{-1/2}|f|^{-1/4}\left\{\cos\left(\frac{2}{3}|\zeta|^{3/2}+\frac{1}{4}\pi\right)+o(1)\right\} \qquad (z\to-\infty), \tag{9.22}$$

where

$$\sigma(z) = \pi^{1/2}\zeta^{1/4}\exp\left(-\frac{2}{3}\zeta^{3/2}\right)\epsilon_2(z). \tag{9.23}$$

An obvious extension of Theorem 2 of the present paper shows that $\sigma(z)$ tends to a finite limit, $\sigma(\infty)$, as $z\to+\infty$. Accordingly

$$w_2(z) = \pi^{-1/2}f^{-1/4}\{1+\sigma(\infty)+o(1)\}\exp\left(\int_0^z f^{1/2}\,dz\right) \qquad (z\to+\infty). \tag{9.24}$$

From (9.20) and the asymptotic form of $M(\zeta)$, we obtain

$$|\sigma(\infty)| \leqslant \frac{1}{2}\sqrt{5}\,\lambda_2\lambda_1^{-1}[\exp\{\lambda_1\mathscr{V}_{-\infty,\infty}(H)\}-1]. \tag{9.25}$$

And with the aid of analysis similar to that used for throwing (9.06) into the form (9.09), we readily show that

$$w_2(z) = \pi^{-1/2}|f|^{-1/4}\{1+o(1)\}\cos\left\{\int_z^0|f|^{1/2}\,dz+\frac{1}{4}\pi+o(1)\right\} \qquad (z\to-\infty). \tag{9.26}$$

Relations (9.24), (9.25), and (9.26) consititute the second Gans-Jeffreys connection formula.

Sharper bounds. Somewhat improved bounds for the error terms of this section can be achieved by application of Theorem 3 of [15],[4] and, in the case of the Bi-type solution, of an inequality of the same character as (3.03) above. The results are expressed by

$$\rho_L \leqslant \exp\{\mathscr{V}_{-\infty,0}(H)+\lambda_4\mathscr{V}_{0,\infty}(H)\}-1, \tag{9.27}$$

and

$$|\sigma(\infty)| \leqslant \exp\left\{\frac{2}{\sqrt{3}}\mathscr{V}_{-\infty,0}(H)+\lambda_5\mathscr{V}_{0,\infty}(H)\right\}-1-\left(\frac{2}{\sqrt{3}}-\frac{1}{2}\right)\mathscr{V}_{-\infty,0}(H), \tag{9.28}$$

where $\lambda_4 = 0.521\ldots$ and $\lambda_5 = 0.520\ldots$.

10. Summary

The primary purpose of this paper has been to investigate approximate solutions of the differential equations (1.01) and, more generally, (4.01) in a complex domain containing no singularities of the functions $f(z)$ and $h(z)$, and a simple zero of $f(z)$. Some preliminary results concerning the Liouville-Green approximation are given in sections 2 through 4. The connection formula for the three fundamental approximations of this kind is then established in section 5, complete with strict error bounds, by considering limiting behavior at the point at infinity. An illustrative application to Airy's differential equation is made in section 6, and some general circumstances in which the error terms vanish are investigated in section 7.

An important special case concerns real variables: the problem here is to connect the exponential-type solutions on one side of the turning point with the oscillatory solutions on the other.

This is solved in section 8 by use of the general formula of section 5. An alternative solution is constructed in section 9 solely from real-variable theory, by re-expansion of known uniform Airy-function approximations. Naturally, different hypotheses on $f(z)$ and $h(z)$ are made in the two methods, but the principal difference lies in the forms of the error bounds. In the first method the bounds depend on the variation of a certain function along an infinite path of specified type in the complex plane. In the second method the bounds depend on the variation of a more complicated function along the real axis.

The error bounds given in this paper have computational applications. As shown in the paper which follows [19], they may also be used to provide theoretical insight into the accuracy of the connection formulas in various circumstances, including cases when the differential equation contains a large parameter. Hitherto, in certain applications it has often been difficult to assess the validity of assumptions which have been made.

11. Addendum

The problems studied in the present paper and its sequel [19] have also been considered in a recent monograph by Fröman and Fröman [20]. These authors have the same principal objective, that is, the determination of strict error bounds for the coefficients in the connection formulas. The method they use resembles the first method of the present paper in that it is a rigorous formulation of the procedure of Zwaan. The difference in the approaches is as follows.

We constructed (in sec. 5) the connection formula for the three fundamental Liouville-Green solutions associated with a simple turning point of the differential equation (4.01) by examining the asymptotic behavior of these solutions in the neighborhood of the point at infinity. Fröman and Fröman, following Kemble [3], express the general solution of (4.01) in the form

$$w(z) = a_1(z) f^{-1/4} \exp\left(\int f^{1/2}\, dz\right) + a_2(z) f^{-1/4} \exp\left(-\int f^{1/2}\, dz\right),$$

and derive a pair of first-order simultaneous differential equations for the functions $a_1(z)$ and $a_2(z)$. These equations are then used to determine the changes in these functions as z passes from one principal subdomain to another. Error bounds for the changes are expressed in terms of contour integrals which are equivalent to the variations of our function $F(z)$.

Generally the path for the contour integrals consists of the real z-axis with indentations bypassing the turning points. Fröman and Fröman show that the appropriate form of monotonicity condition is fulfilled when the indentations are semicircles of sufficiently small radius ([20], p. 39). Owing to the singularities of $F(z)$ at the turning points however, the error bounds tend to infinity as the indentations shrink to zero. In consequence Fröman and Fröman assume that the indentations can actually be taken sufficiently large to yield small error bounds, without violating the monotonicity condition. In the present paper we allow greater flexibility in the choice of paths, with a view to achieving minimum bounds in applications.

Other comparisons with the first method of the present paper are as follows:

(i) There is greater emphasis in [20] on the case in which the coefficients $f(z)$ and $h(z)$ in the differential equation (4.01) are real on the real axis.

(ii) Approximations and expansions are frequently used in [20] to simplify the error bounds. There is greater emphasis on strict bounds in the present paper and [19].

(iii) In the special limiting case in which z is at infinity the error bounds can be sharpened by a factor of 2 (see Theorem 2 of sec. 3 above). This refinement is freely used in the present paper and [19], but is not in evidence in [20].

The author acknowledges helpful criticisms of the draft of this paper by Drs. J. Heading, L. Maximon, and F. Stenger.

The work described above has been supported by the U.S. Army Research Office, Durham, North Carolina (Project No. 4238-M).

12. References

[1] Olver, F. W. J., Error bounds for the Liouville-Green (or WKB) approximation, Proc. Camb. Phil. Soc. **57**, 790–810 (1961).

[2] Zwaan, A., Intensitäten im *Ca*-Funkenspektrum, Arch. Néerlandaises des Sciences Exactes, Ser. 3A **12**, 1–76 (1929).

[3] Kemble, E. C., A contribution to the theory of the BWK method, Phys. Rev. **48**, 549–561 (1935).

[4] Furry, W. H., Two notes on phase-integral methods, Phys. Rev. **71**, 360–371 (1947).

[5] Gans, R., Fortpflanzung des Lichts durch ein inhomogenes Medium, Ann. Phys. Lpz. **47**, 709–736 (1915).

[6] Jeffreys, H., On certain approximate solutions of linear differential equations of the second order, Proc. Lond. Math. Soc. (2) **23**, 428–436 (1924–5).

[7] Kramers, H. A., Wellenmechanik und halbzahlige Quantisierung, Z. Phys. **39**, 828–840 (1926).

[8] Langer, R. E., On the connection formulas and the solutions of the wave equation, Phys. Rev. **51**, 669–676 (1937).

[9] Jeffreys, H., On approximate solutions of linear differential equations, Proc. Camb. Phil. Soc. **49**, 601–611 (1953).

[10] Jeffreys, H., Asymptotic approximations (Oxford University Press, 1962).

[11] Morse, P. M. and Feshbach, H., Methods of theoretical physics, Pt 2 (McGraw-Hill Book Co., Inc., New York, N.Y. 1953).

[12] Budden, K. G., Radio waves in the ionosphere. (Cambridge University Press, 1961).

[13] Heading, J., An introduction to phase-integral methods, (John Wiley & Sons, Inc., New York, N.Y., 1962).

[14] Langer, R. E., The asymptotic solutions of ordinary linear differential equations of the second order, with special reference to the Stokes phenomenon, Bull. Amer. Math. Soc. **40**, 545–582 (1934).

[15] Olver, F. W. J., Error bounds for first approximations in turning-point problems, J. Soc. Indust. Appl. Math. **11**, 748–772 (1963).

[16] Olver, F. W. J., Uniform asymptotic expansions of solutions of linear second-order differential equations for large values of a parameter, Phil. Trans. Roy. Soc. London, Ser. A **250**, 479–517 (1958).

[17] Olver, F. W. J., On the asymptotic solutions of second-order differential equations having an irregular singularity of rank one, with an application to Whittaker functions, J. Soc. Indust. Appl. Math. Ser. B **2**, 225–243 (1965).

[18] Miller, J. C. P., The Airy Integral, Brit. Ass. Math. Tab. Part–Vol. B. (Cambridge University Press, 1946).

[19] Olver, F. W. J., Error analysis of phase-integral methods. II. Application to wave-penetration problems, J. Res. NBS **69B**, No. 4, 291–300 (1965).

[20] Fröman, N. and Fröman, P. O., JWKB approximation-Contributions to the theory (North-Holland Publishing Co., Amsterdam, 1965).

(Paper 69B4–157)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 69B, No. 4, October–December 1965

Error Analysis of Phase-Integral Methods. II. Application to Wave-Penetration Problems

F. W. J. Olver

(July 1, 1965)

A study is made of the differential equation

$$d^2w/dz^2 = \{f(z) + h(z)\}w,$$

in which $f(z)$ and $h(z)$ are real and regular on the real axis, and $f(z)$ has exactly two zeros there. Strict error bounds are derived for the coefficients in the formulas which connect the asymptotic solutions at $z = +\infty$ with the asymptotic solutions at $z = -\infty$. Applications are made to two physical problems.

Key Words: Wave penetration, connection formulas, error bounds, potential barrier, transmission coefficient, harmonic oscillator.

1. Introduction and Summary

The purpose of this paper is to illustrate the theory of the preceding paper [1][1] with two problems arising from the one-dimensional wave equation

$$\frac{d^2w}{dz^2} = \{f(z) + h(z)\}w. \tag{1.01}$$

In both problems the functions $f(z)$ and $h(z)$ are real when z is real, and in the region considered $f(z)$ has no singularities and just two zeros, both of which are real and simple. The function $h(z)$ is to be regarded in some sense as being small compared with $f(z)$, but we do not need to formulate this assumption precisely at the outset.

In the first problem (secs. 2, 3) $f(z)$ is positive between the zeros. The object is to determine the ratio of the amplitude of an oscillatory solution at $z = +\infty$ to the amplitudes of its components at $z = -\infty$.

In the second problem (secs. 4, 5) $f(z)$ is negative between the zeros. The object here is to determine eigenconditions admitting a solution having subdominant (exponentially small) character at both $-\infty$ and $+\infty$.

Both problems have been treated frequently in the literature; see the references cited in [1], and [2]–[7] given at the end of this paper. Generally, the viewpoint adopted has been that $f(z)$ contains a multiplicative factor u^2, $h(z)$ is independent of u, and approximate solutions are sought which are asymptotically correct for large values of the parameter u. In the present paper, we establish explicit strict error bounds for the approximate solutions. Asymptotic properties with respect to parameters are immediate consequences of the forms of the bounds.

Two methods for solution were given in [1]. We shall concentrate on the first (Zwaan's method). As we shall see, from the standpoint of deriving error bounds this affords the simpler approach to the present problems.

2. The Overdense Potential Barrier

In this section we suppose that $f(z)$ and $h(z)$ are regular in an unbounded, simply connected complex domain $\mathbf{D}$, which includes the whole of the real axis, and that the only zeros of $f(z)$ in $\mathbf{D}$ are simple zeros at $z = \pm a$ $(a > 0)$. When $-a < z < a$, $f(z)$ is positive.

[1] Figures in brackets indicate the literature references at the end of this paper.

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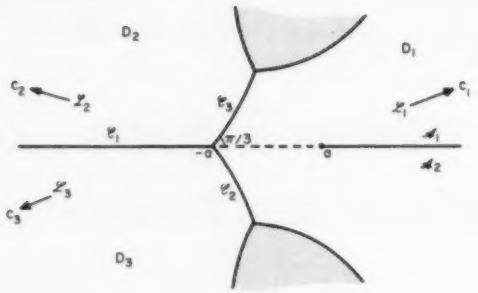

FIGURE 1. *Typical principal subdomains for the overdense potential barrier.*

Let us consider the turning point at $z=-a$. In order to apply the theory of [1], section 5, we have to exclude the other zero $z=a$ from the domain of consideration, and we do this by introducing a cut $\mathscr{A}$ along the real axis from $z=a$ to $z=+\infty$. We shall refer to the upper and lower sides of this cut as $\mathscr{A}_1$ and $\mathscr{A}_2$, respectively. As in [1], section 5, we define

$$\xi(z)=\int_{-a}^{z}\{f(t)\}^{1/2}dt. \tag{2.01}$$

The associated principal curves $\mathscr{C}_j$ and subdomains $\mathbf{D}_j$ are indicated in figure 1. $\mathscr{C}_1$ is the part of the real axis which extends from $-a$ to $-\infty$. $\mathscr{C}_2, \mathscr{C}_3$ are conjugate curves emerging from $-a$ at directions $\mp\pi/3$. They cannot intersect the real axis at any other point. We define $\xi_j(z)$ to be the branch of $\xi(z)$ which is continuous in $\mathbf{D}$ cut along $\mathscr{A}$ and $\mathscr{C}_j$, and has positive real part in $\mathbf{D}_j$. Similarly, $g_1(z)$, $g_2(z)$, $g_3(z)$ are multiples of any branches of $g(z)\equiv\{f(z)\}^{-1/4}$ which are continuous in $\mathbf{D}$ cut along $\mathscr{A}$ and the corresponding $\mathscr{C}_j$, and satisfy eq (5.08) of [1].

As in [1], let c_j be points at infinity on arbitrary ξ-progressive curves $\mathscr{L}_j$ lying within $\mathbf{D}_j$ such that $|\mathrm{Re}\ \xi(c_j)|=\infty$. $\mathscr{L}_1$ is taken in the upper half-plane, and $\mathscr{L}_2$, $\mathscr{L}_3$ are complex conjugates, but no boundary of $\mathbf{D}$ may intervene between $\mathscr{L}_2$ and $\mathscr{L}_3$ in the neighborhood of infinity. The other assumptions we make are

(i) The variation of the function

$$F\equiv\int\left\{\frac{h}{f^{1/2}}-\frac{1}{f^{1/4}}\frac{d^2}{dz^2}\left(\frac{1}{f^{1/4}}\right)\right\}dz \tag{2.02}$$

converges as $z\to c_j$ along $\mathscr{L}_j$, and also as $z\to\pm\infty$ along the real axis.

(ii) ξ-progressive curves can be found in $\mathbf{D}$ linking: (a) c_1 with c_2; (b) c_1 with c_3; (c) c_2 or c_3 with any point of the interval $(-\infty,-a)$; (d) c_1 with any point of $\mathscr{A}_1$.

(iii) $\epsilon_2(c_3)=0$; $\epsilon_2(z)$ and $\epsilon_3(z)\to 0$ as $z\to-\infty$; $\epsilon_1(z)\to 0$ as $z\to+\infty$ on $\mathscr{A}_1$.

(A brief discussion of the determination of ξ-progressive paths is given in the remark at the end of [1], sec. 5, and sufficient conditions for the fulfillment of (iii) are given in sec. 7 of the same paper.)

With these conditions, the fundamental connection formula ([1], sec. 5) for the solutions

$$w_j(z)=g_j(z)e^{-\xi_j(z)}\{1+\epsilon_j(z)\} \tag{2.03}$$

of the differential eq (1.01), becomes

$$w_1(z)=e^{\pi i/3}\{1+\epsilon_1(c_3)\}w_2(z)+e^{-\pi i/3}\{1+\epsilon_1(c_2)\}w_3(z). \tag{2.04}$$

We fix the $w_j(z)$ by specifying that $g_1(z)$ is the branch of $\{f(z)\}^{-1/4}$ which takes its principal value on the join of $-a$ and $+a$, and interpret the branches of the two sides of (2.04) in real form, as follows.

When $z \in \mathscr{A}_1$, we have

$$\xi_1(z) = \alpha - i\int_a^z |f|^{1/2}dt, \qquad g_1(z) = e^{\pi i/4}|f|^{-1/4}, \tag{2.05}$$

where

$$\alpha = \int_{-a}^{a} |f|^{1/2}dt \tag{2.06}$$

and is positive. Therefore from (2.03) and hypothesis (iii)

$$w_1(z) = e^{-\alpha}|f|^{-1/4}\{1+o(1)\}\ \exp\Big(i\int_a^z |f|^{1/2}dt + \frac{1}{4}\pi i\Big) \qquad (z \to +\infty). \tag{2.07}$$

This expression represents a *transmitted wave* ([8], p. 1100; [6]).

When $-\infty < z < -a$, we have

$$\xi_2(z) = i\int_z^{-a} |f|^{1/2}dt, \qquad g_2(z) = e^{-\pi i/12}|f|^{-1/4}. \tag{2.08}$$

Hence

$$e^{\pi i/3}\{1+\epsilon_1(c_3)\}w_2(z) = |f|^{-1/4}\{1+\epsilon_1(c_3)+o(1)\}\ \exp\Big(-i\int_z^{-a} |f|^{1/2}dt + \frac{1}{4}\pi i\Big) \qquad (z \to -\infty). \tag{2.09}$$

This is the *incident wave*, moving in the same direction as the transmitted wave. Similarly

$$e^{-\pi i/3}\{1+\epsilon_1(c_2)\}w_3(z) = |f|^{-1/4}\{1+\epsilon_1(c_2)+o(1)\}\ \exp\Big(i\int_z^{-a} |f|^{1/2}dt - \frac{1}{4}\pi i\Big) \qquad (z \to -\infty). \tag{2.10}$$

This is the *reflected wave*, moving in the opposite direction to the transmitted wave.

The *transmission coefficient* [2] T and the *reflection coefficient* R are the squares of the limiting ratios of the wave amplitudes. Thus

$$T = e^{-2\alpha}|1+\epsilon_1(c_3)|^{-2}, \tag{2.11}$$

$$R = |1+\epsilon_1(c_2)|^2|1+\epsilon_1(c_3)|^{-2}, \tag{2.12}$$

where ([1], (5.17))

$$|\epsilon_1(c_j)| \leqslant \tfrac{1}{2}\ \exp\{\mathscr{V}_{c_1,c_j}(F)\} - \tfrac{1}{2} \qquad (j=2,3), \tag{2.13}$$

the variations being evaluated along ξ-progressive curves.

Alternative, and sometimes more effective, formulas for T and, especially, R, can be derived with the aid of the energy-conservation eq ([8], p. 1066; [9], sec. 4.4)

$$T + R = 1. \tag{2.14}$$

[2] Or "tunnelling probability" [7].

(This relation may be verified analytically by means of Theorem 4 of [10] and the Wronskian property of the solutions of the differential equation.) Substitution of (2.11) and (2.12) in (2.14) yields

$$|1+\epsilon_1(c_3)|^2-|1+\epsilon_1(c_2)|^2=e^{-2a}. \tag{2.15}$$

Hence

$$T=\frac{e^{-2a}}{|1+\epsilon_1(c_2)|^2+e^{-2a}}, \tag{2.16}$$

$$R=1-\frac{e^{-2a}}{|1+\epsilon_1(c_3)|^2}=\frac{|1+\epsilon_1(c_2)|^2}{|1+\epsilon_1(c_2)|^2+e^{-2a}}. \tag{2.17}$$

Remark. It is interesting to observe that we have not used the connection formula for the turning point at $z=+a$. In contrast, if the problem of this section were attacked by real-variable theory ([1], sec. 9) connection formulas at both $-a$ and $+a$ would have to be used, and the resulting approximate solutions of the differential equation then matched in the interval $-a<z<a$; see, for example, [5, 6].[3] The error analysis obviously would be lengthier and lead to more complicated bounds.

3. Example [4]

Consider the modified Weber equation

$$d^2w/dz^2=(a^2-z^2)w \qquad (a>0). \tag{3.01}$$

We take $f(z)=a^2-z^2$ and $h(z)=0$. Then

$$\xi(z)=\int_{-a}^{z}(a^2-t^2)^{1/2}dt=\tfrac{1}{2}\pi a^2-\tfrac{1}{2}a^2\cos^{-1}(z/a)+\tfrac{1}{2}z(a^2-z^2)^{1/2}. \tag{3.02}$$

The principal subdomains in the z-plane are shown in figure 2 (compare [12], sec. 3). The

[3] A real-variable method which avoids this matching has been suggested by Miller and Good [4] and by Pike [7], but it has yet to be placed on a firm mathematical foundation.

[4] For an account of some direct numerical calculations of transmission coefficients to high precision see [11].

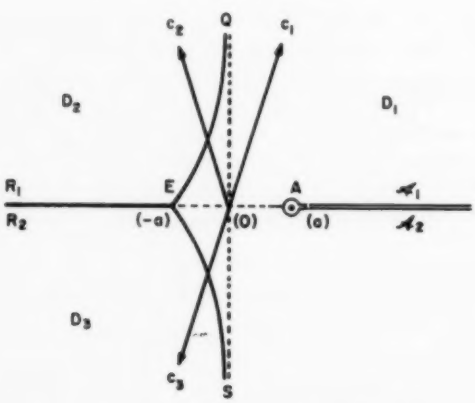

FIGURE 2. *z-plane: principal subdomains.*

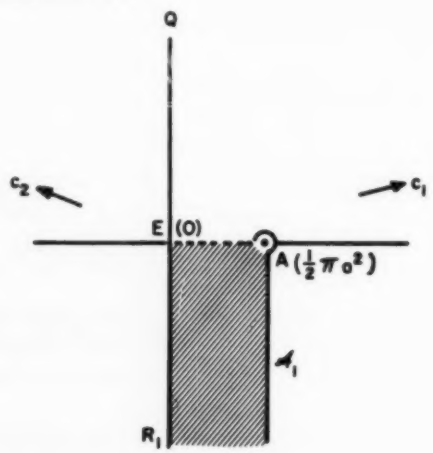

FIGURE 3. *ξ_1-plane.*

corresponding map of the upper half of the z-plane on the ξ_1-plane is indicated in figure 3; the map of the lower half is of course the image of figure 3 in the real axis.

The reference points c_1, c_2, and c_3 are taken at infinity on outward-drawn rays from the origin in the first, second, and third quadrants of the z-plane, respectively. With the aid of the ξ_1-map, we see immediately that hypotheses (i) and (ii) of section 2 are satisfied. Theorem 4 of [1] shows that hypothesis (iii) is satisfied, and also that $\epsilon_1(c_2)=0$. From the definition (2.06) we have $\alpha=\frac{1}{2}\pi a^2$. Hence from eqs (2.16) and (2.17), we derive

$$T=\frac{e^{-\pi a^2}}{1+e^{-\pi a^2}}, \qquad R=\frac{1}{1+e^{-\pi a^2}}. \tag{3.03}$$

These results may be verified analytically with the aid of asymptotic expansions and connection formulas for the Weber functions given, for example, in [13]. The actual expression for $w_1(z)$ is found to be, in Miller's notation,

$$w_1(z)=2^{-(ia^2+1)/4}a^{ia^2/2}\exp\left(-\frac{1}{2}\pi a^2-\frac{1}{4}ia^2-\frac{1}{2}i\varphi_2\right)\left\{k^{-1/2}W\left(\frac{1}{2}a^2,\sqrt{2}z\right)+ik^{1/2}W\left(\frac{1}{2}a^2,-\sqrt{2}z\right)\right\}. \tag{3.04}$$

It is noteworthy that our theory [5] proves sufficiently powerful to yield exact expressions for T and R. This example, however, is unique in this respect.

4. The Approximate Harmonic Oscillator

The conditions assumed in this section are those stated in the opening paragraph of section 2, except that $f(z)$ is negative when $-a<z<a$.

We distinguish the auxiliary functions and principal subdomains associated with the turning point at $z=-a$ from those associated with $z=+a$ by the addition of tildes. Thus

$$\xi(z)=\int_a^z\{f(t)\}^{1/2}dt, \qquad \tilde{\xi}(z)=\int_{-a}^z\{f(t)\}^{1/2}dt. \tag{4.01}$$

Three principal curves emerge from $-a$ and three from $+a$, one of which in each case is the join of $-a$ and $+a$; see figure 4. Let $\mathbf{D}_1$, $\tilde{\mathbf{D}}_1$ be the principal subdomains which include the points

[5] This is also true of the theory of [14], section 9.1.

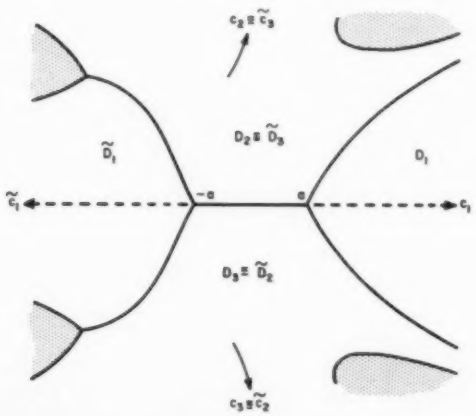

FIGURE 4. *Typical principal subdomains for the approximate harmonic oscillator.*

$c_1 \equiv +\infty$ and $\bar{c}_1 \equiv -\infty$, respectively. Then clearly $\bar{\mathbf{D}}_2 \equiv \mathbf{D}_3$ and $\bar{\mathbf{D}}_3 \equiv \mathbf{D}_2$. We take c_2, c_3 to be points at infinity on conjugate ξ-progressive curves lying within $\mathbf{D}_2$, $\mathbf{D}_3$, respectively, and $\bar{c}_2 = c_3$, $\bar{c}_3 = c_2$. We assume that ξ-progressive curves can be found in $\mathbf{D}$ linking c_2 and c_3 with $+\infty$ and $-\infty$, and also with each other, and that $|\mathrm{Re}\ \xi(z)| \to \infty$ as z tends to any of the c_j or $\bar{c}_j$.

The fundamental connection formulas for the two turning points are given by

$$\{1+\epsilon_2(c_3)\}w_1(z)+e^{-2\pi i/3}\{1+\epsilon_3(c_1)\}w_2(z)+e^{2\pi i/3}\{1+\epsilon_1(c_2)\}w_3(z)=0, \tag{4.02}$$

and

$$\{1+\bar{\epsilon}_2(\bar{c}_3)\}\bar{w}_1(z)+e^{-2\pi i/3}\{1+\bar{\epsilon}_3(\bar{c}_1)\}\bar{w}_2(z)+e^{2\pi i/3}\{1+\bar{\epsilon}_1(\bar{c}_2)\}\bar{w}_3(z)=0. \tag{4.03}$$

Clearly $\bar{w}_3(z)$ is a multiple of $w_2(z)$, and $\bar{w}_2(z)$ a multiple of $w_3(z)$. To fix these relationships we suppose that $g_1(z)$ and $\bar{g}_1(z)$ are the branches of the function $\{f(z)\}^{-1/4}$ which take their principal values when $z > a$ and $z < -a$, respectively. We then find that if $z \in \mathbf{D}_2$

$$\xi_2(z) = i\alpha + \bar{\xi}_3(z), \qquad g_2(z) = e^{-\pi i/6}\bar{g}_3(z), \tag{4.04}$$

where α is again defined by (2.06). Therefore

$$\bar{w}_3(z) = e^{(\pi i/6)+i\alpha}\, w_2(z), \qquad \bar{\epsilon}_3(z) = \epsilon_2(z). \tag{4.05}$$

Substituting these and the corresponding results for $\bar{w}_2(z)$ and $\bar{\epsilon}_2(z)$ in (4.03), we obtain the connection formula for $\bar{w}_1(z)$, $w_2(z)$ and $w_3(z)$. Elimination of $w_3(z)$ by means of (4.02) then yields

$$w_1(z) = \left[\frac{1+\epsilon_1(c_3)}{1+\epsilon_2(c_3)} + \frac{\{1+\epsilon_1(c_2)\}\{1+\bar{\epsilon}_1(c_3)\}}{\{1+\epsilon_2(c_3)\}\{1+\bar{\epsilon}_1(c_2)\}}\, e^{2i\alpha}\right] e^{\pi i/3} w_2(z) - \frac{1+\epsilon_1(c_2)}{1+\bar{\epsilon}_1(c_2)}\, i e^{i\alpha}\bar{w}_1(z). \tag{4.06}$$

The eigencondition or "quantization condition" is that $w_1(z)$ be a multiple of $\bar{w}_1(z)$. Accordingly, this is expressed by

$$e^{2i\alpha} = -\frac{\{1+\epsilon_1(c_3)\}\{1+\bar{\epsilon}_1(c_2)\}}{\{1+\epsilon_1(c_2)\}\{1+\bar{\epsilon}_1(c_3)\}}. \tag{4.07}$$

Neglecting the error terms, we obtain at once the well-known approximations $\alpha = \frac{1}{2}\pi, \frac{3}{2}\pi, \frac{5}{2}\pi, \ldots$. To assess the errors in these approximations, we write

$$\epsilon_1(c_3) = pe^{iq}, \qquad \epsilon_1(c_2) = pe^{-iq}, \qquad \bar{\epsilon}_1(c_2) = \bar{p}e^{i\bar{q}}, \qquad \bar{\epsilon}_1(c_3) = \bar{p}e^{-i\bar{q}}, \tag{4.08}$$

where $p, \bar{p} > 0$ and $q, \bar{q}$ are real. Then

$$\ln\left[\frac{\{1+\epsilon_1(c_3)\}\{1+\bar{\epsilon}_1(c_2)\}}{\{1+\epsilon_1(c_2)\}\{1+\bar{\epsilon}_1(c_3)\}}\right] = 2i(\omega+\bar{\omega}), \tag{4.09}$$

where $\omega, \bar{\omega}$ are real, and

$$|\omega| \leqslant \sin^{-1} p \leqslant \tfrac{1}{2}\pi p, \qquad |\bar{\omega}| \leqslant \sin^{-1}\bar{p} \leqslant \tfrac{1}{2}\pi\bar{p}, \tag{4.10}$$

provided that $p, \bar{p} \leqslant 1$. Hence the eigencondition is given by

$$\alpha = (n + \tfrac{1}{2} + \beta)\pi \qquad (n = 0, 1, 2, \ldots), \tag{4.11}$$

where $\beta=(\omega+\bar{\omega})/\pi$ and is real. From (4.08), (4.10) and [1], (5.17), we obtain the desired bound

$$|\beta| \leqslant \frac{1}{4}\exp\{\mathcal{V}_{x,c_2}(F)\}+\frac{1}{4}\exp\{\mathcal{V}_{-\infty,c_2}(F)\}-\frac{1}{2}, \tag{4.12}$$

where F is any continuous branch of the integral defined by (2.02) above, and the variations are taken along ξ-progressive paths.

When the eigencondition is satisfied, eq (4.06) reduces to

$$w_1(z)=(-)^n\frac{1+\delta}{1+\bar{\delta}}\,\bar{w}_1(z), \tag{4.13}$$

where

$$|\delta| \leqslant \tfrac{1}{2}\exp\{\mathcal{V}_{x,c_2}(F)\}-\tfrac{1}{2}, \qquad |\bar{\delta}| \leqslant \tfrac{1}{2}\exp\{\mathcal{V}_{-\infty,c_2}(F)\}-\tfrac{1}{2}. \tag{4.14}$$

Thus on the real axis the eigensolution is given by

$$w_1(z)=\{1+\epsilon_1(z)\}f^{-1/4}\exp\left(-\int_a^z f^{1/2}dt\right), \tag{4.15}$$

where

$$|\epsilon_1(z)| \leqslant \exp\{\mathcal{V}_{x,z}(F)\}-1 \qquad (z>a), \tag{4.16}$$

and

$$w_1(z)=(-)^n(1+\delta)(1+\bar{\delta})^{-1}\{1+\bar{\epsilon}_1(z)\}f^{-1/4}\exp\left(-\int_z^{-a} f^{1/2}dt\right), \tag{4.17}$$

where

$$|\bar{\epsilon}_1(z)| \leqslant \exp\{\mathcal{V}_{-x,z}(F)\}-1 \qquad (z<-a). \tag{4.18}$$

The fractional powers in (4.15) and (4.17) are positive, and the variations in (4.16) and (4.18) are taken along the real axis.

Remark. Let $f(z)$ and $h(z)$ be even functions of z, and assume that c_2, c_3 can be taken as the points $\pm i\infty$. Then the bound (4.12) and eq (4.13) reduce to

$$|\beta| \leqslant \tfrac{1}{2}\exp\{\mathcal{V}_{x,ix}(F)\}-\tfrac{1}{2}, \tag{4.19}$$

and

$$w_1(z)=(-)^n\bar{w}_1(z)=(-)^n w_1(-z). \tag{4.20}$$

5. Examples

(i) *Weber equation.*

$$d^2w/dz^2=(z^2-a^2)w \qquad (a>0). \tag{5.01}$$

We take $f(z)=z^2-a^2$ and $h(z)=0$. Then

$$\xi(z)=\int_a^z (t^2-a^2)^{1/2}dt=\tfrac{1}{2}z(z^2-a^2)^{1/2}-\tfrac{1}{2}a^2\ln\{z+(z^2-a^2)^{1/2}\}+\tfrac{1}{2}a^2\ln a. \tag{5.02}$$

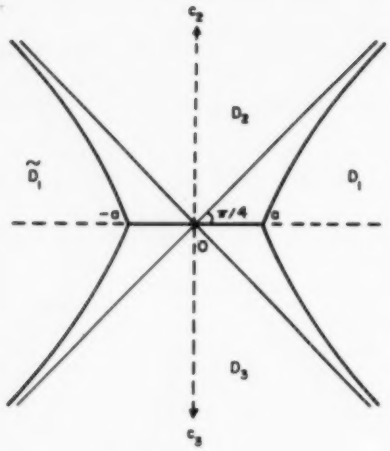

FIGURE 5. *Principal subdomains for the Weber equation.*

Figure 5 illustrates the principal subdomains. We take c_2, c_3 to be the points $\pm i\infty$. From [1], theorem 4, we see that $\epsilon_1(c_2)=\tilde{\epsilon}_1(c_2)=0$. Hence in (4.08) $p=\tilde{p}=0$. Therefore β vanishes and $\alpha=(n+\frac{1}{2})\pi$, *exactly*.[6] Using (2.06), we see that this implies $a^2=2n+1$. The eigensolution of course obeys (4.20). These results accord with the known analytical properties of the Weber functions [13].

(ii) *Large parameter.* Let $f(z)=u^2f_0(z)$, where u is a large positive parameter, and the functions $f_0(z)$ and $h(z)$ are independent of u (though this restriction could be eased without significantly affecting the following analysis). Then

$$\alpha=u\alpha_0, \qquad F(z)=F_0(z)/u, \tag{5.03}$$

where

$$\alpha_0=\int_{-a}^{a}|f_0|^{1/2}dt, \qquad F_0(z)=\int\left\{\frac{h}{f_0^{1/2}}-\frac{1}{f_0^{1/4}}\frac{d^2}{dz^2}\left(\frac{1}{f_0^{1/4}}\right)\right\}dz, \tag{5.04}$$

and are independent of u. Write

$$\chi(u)\equiv\frac{1}{4}\exp\{u^{-1}\mathscr{V}_{\infty,c_2}(F_0)\}+\frac{1}{4}\exp\{u^{-1}\mathscr{V}_{-\infty,c_2}(F_0)\}-\frac{1}{2}. \tag{5.05}$$

Then the eigencondition (4.11) is expressed by the following equation for u:

$$\psi(u)\equiv u\alpha_0-(n+\tfrac{1}{2})\pi-\pi\beta(u)=0, \tag{5.06}$$

in which

$$|\beta(u)|\leq\chi(u). \tag{5.07}$$

For large u, $\chi(u)=O(u^{-1})$. Therefore for large values of the positive integer n

$$u=\alpha_0^{-1}(n+\tfrac{1}{2})\pi+O(n^{-1}). \tag{5.08}$$

[6] Compare also [14], page 109.

In order to determine precise bounds for the O term in the last equation, consider the function $\chi(u)$. This tends to infinity as $u \to 0$, and to zero as $u \to \infty$, and is monotonic strictly decreasing when u is positive. Let u_0 be the root of $\chi(u_0) = \frac{1}{2}$. Then provided that $n\pi/\alpha_0 > u_0$, we have from (5.06) and (5.07)

$$\psi(n\pi/\alpha_0) = -\tfrac{1}{2}\pi - \pi\beta(n\pi/\alpha_0) < 0, \tag{5.09}$$

and

$$\psi\{(n+1)\pi/\alpha_0\} = \tfrac{1}{2}\pi - \pi\beta\{(n+1)\pi/\alpha_0\} > 0. \tag{5.10}$$

Therefore at least one eigenvalue exists in the interval $n\pi/\alpha_0 < u < (n+1)\pi/\alpha_0$. To delimit it in a shorter interval, let

$$u = (n + \tfrac{1}{2} + v)\pi/\alpha_0, \tag{5.11}$$

where $|v| < \frac{1}{2}$. Then substituting in (5.06), we obtain

$$v = \beta\{(n + \tfrac{1}{2} + v)\pi/\alpha_0\}. \tag{5.12}$$

Hence $|v| < \chi(n\pi/\alpha_0)$, that is,

$$|v| < \frac{1}{4}\exp\left\{\frac{\alpha_0}{n\pi}\,\mathcal{V}_{\infty,\,c_2}(F_0)\right\} + \frac{1}{4}\exp\left\{\frac{\alpha_0}{n\pi}\,\mathcal{V}_{-\infty,\,c_2}(F_0)\right\} - \frac{1}{2}. \tag{5.13}$$

Relations (5.11) and (5.13) constitute the precise form of the eigencondition (5.08), and are valid when $n > \alpha_0 u_0/\pi$. The eigensolution satisfies (4.13), where

$$|\delta| \leqslant \frac{1}{2}\exp\left\{\frac{\alpha_0}{n\pi}\,\mathcal{V}_{\infty,\,c_2}(F_0)\right\} - \frac{1}{2}, \qquad |\tilde{\delta}| \leqslant \frac{1}{2}\exp\left\{\frac{\alpha_0}{n\pi}\,\mathcal{V}_{-\infty,\,c_2}(F_0)\right\} - \frac{1}{2}. \tag{5.14}$$

The above proof shows that there is at least one eigenvalue (5.11) which satisfies (5.13). In order to establish that there is *exactly* one eigenvalue of this form, we need to investigate the sign of the derivative $\beta'(u)$ in the interval considered.[7] This takes us back to fundamentals. We have to consider the Liouville-Green approximate solutions of the differential equation

$$d^2w/dz^2 = \{u^2 + f(z)\}w \tag{5.15}$$

(compare [1], sec. 2) as functions of u, and seek bounds for the u-derivatives of their error terms. The analysis is somewhat lengthy, and we record only the result:

Let

$$X(u) = \frac{le^{l}}{3-e^{l}}\,\frac{1+\kappa}{u} + \frac{\bar{l}e^{\bar{l}}}{3-e^{\bar{l}}}\,\frac{1+\bar{\kappa}}{u} - \alpha_0, \tag{5.16}$$

where

$$l = u^{-1}\mathcal{V}_{\infty,\,c_2}(F_0), \qquad \bar{l} = u^{-1}\mathcal{V}_{-\infty,\,c_2}(F_0), \tag{5.17}$$

$$\kappa = (2e\cos\gamma)^{-1}, \qquad \bar{\kappa} = (2e\cos\bar{\gamma})^{-1}, \tag{5.18}$$

[7] An alternative, but apparently no easier, approach would be to consider complex values of u and apply Rouché's theorem.

and γ, $\tilde{\gamma}$ are the maximum angles of slope with the real ξ-axis of the ξ-maps of the progressive paths linking ∞ to c_2, and $-\infty$ to c_2, respectively ($|\gamma|$, $|\tilde{\gamma}| < \frac{1}{2}\pi$). Then exactly one eigenvalue satisfies (5.11) and (5.13), provided that $n \geqslant \alpha_0 u_1/\pi$ where u_1 is the largest positive zero of $X(u)$.

Some simplification can be effected by using upper bounds for the zeros of $\chi(u) - \frac{1}{2}$ and $X(u)$. In this way we may verify that both of the conditions $n > \alpha_0 u_0/\pi$ and $n \geqslant \alpha_0 u_1/\pi$ are certainly fulfilled if n exceeds each of the three quantities

$$\frac{\alpha_0 \mathcal{J}_{\infty, c_2}(F_0)}{\pi \ln 2}, \qquad \frac{\alpha_0 \mathcal{J}_{-\infty, c_2}(F_0)}{\pi \ln 2}, \qquad \frac{2 \ln 2}{\pi}(2 + \kappa + \tilde{\kappa}). \tag{5.19}$$

The author acknowledges helpful criticisms of the draft of this paper by Drs. J. Heading and L. Maximon.

The work described above has been supported by the U.S. Army Research Office, Durham, N. Carolina (Project No. 4238-M).

6. References

[1] Olver F. W. J., Error analysis of phase-integral methods. I. General theory for simple turning points, J. Res. NBS **69B**, No. 4, 271–290 (1965).

[2] Dunham, J. L., The Wentzel-Brillouin-Kramers method of solving the wave equation, Phys. Rev. **41**, 713–720 (1932).

[3] Birkhoff, G. D., Quantum mechanics and asymptotic series. Bull. Amer. Math. Soc. **39**, 681–700 (1933).

[4] Miller, S. C., and Good, R. H., A WKB-type approximation to the Schrödinger equation, Phys. Rev. **91**, 174–179 (1953).

[5] Jeffreys, H., On the use of asymptotic approximations of Green's type when the coefficient has zeros, Proc. Camb. Phil. Soc. **52**, 61–66 (1956).

[6] McLeod, J. B., The determination of the transmission coefficient, Quart. J. Math. Oxford (2) **12**, 153–158 (1961).

[7] Pike, E. R., On the related-equation method of asymptotic approximation II. Direct solutions of wave-penetration problems, Quart. J. Mech. Appl. Math. **17**, 369–379 (1964).

[8] Morse, P. M., and Feshbach, H., Methods of Theoretical Physics, Pt 2 (McGraw-Hill Book Co., Inc., New York, N.Y., 1953).

[9] Heading, J., An Introduction to Phase-Integral Methods (John Wiley & Sons, Inc., New York, N.Y., 1962).

[10] Olver, F. W. J., Error bounds for the Liouville-Green (or WKB) approximation, Proc. Camb. Phil. Soc. **57**, 790–810 (1961).

[11] Jamet, P., Calcul exact du coefficient de transmission d'une barrière de potentiel: étude de l'erreur de l'approximation BKW (in press).

[12] Olver, F. W. J., Uniform asymptotic expansions for Weber parabolic cylinder functions of large orders, J. Res. NBS **63B** (Math. and Math. Phys.), No. 2, 131–169 (1959).

[13] Miller, J. C. P., Tables of Weber parabolic cylinder functions (Her Majesty's Stationery Office, London, 1955).

[14] Fröman, N., and Fröman, P. O., JWKB approximation—Contributions to the theory (North-Holland Publishing Co., Amsterdam, 1965).

(Paper 69B4–158)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 69B, No. 4, October–December 1965

A Random Walk Model of Chain Polymer Adsorption at a Surface. II. Effect of Correlation Between Neighboring Steps

Robert J. Rubin

(July 21, 1965)

A random walk lattice model of adsorption of an isolated polymer chain at a solution surface is investigated. The model is a modification of a simple cubic lattice in which there is a correlation between successive steps. The direction of each step is at right angles to the direction of the preceding step (all bond angles are 90°). One-dimensional characteristics of the monomer unit distribution are determined analytically in the limit of long polymer chains neglecting the self-excluded volume. The mean number of monomer units adsorbed in the surface layer $\nu(\theta, N)$ is determined assuming that one end of the polymer chain lies in the surface layer, where N is the mean number of monomer units in the chain and θ is the adsorption energy of each monomer unit in the surface layer measured in units of kT. In addition, the mean distance of the free end of the chain from the surface layer $z(\theta, N)$ is determined. The properties of this correlated step model are qualitatively similar to the properties which have been found in uncorrelated step models. In particular, there is a critical value of the adsorption energy θ_c such that for $\theta > \theta_c$, $\nu(\theta, N)$ is proportional to N. Numerical values of $N^{-1}\nu(\theta, N)$ and $z(\theta, N)$ are presented for $\theta > \theta_c = \ln(\sqrt{5}-1)$.

Key Words: Chain polymer, adsorption, random walk, lattice model, short range correlation, critical energy, partition function, generating function.

1. Introduction

We have recently studied a variety of random walk lattice models of polymer chain adsorption at a solution surface [1].[1] At the same time F. McCrackin [2] has completed a Monte Carlo investigation of still another lattice model of polymer chain adsorption at a solution surface in which he treats the effect of the self-excluded volume of the polymer chain. The lattice model treated by McCrackin is a simple cubic lattice in which the direction of each step must be at right angles to the direction of the preceding step. Thus there is a correlation between neighboring steps in his model. The purpose of this paper is twofold: (1) To generalize the methods developed in I in order to treat a lattice model with correlation between neighboring steps, and (2) to determine some of the moments of the monomer unit distribution which will serve as reference values for the excluded volume computations of McCrackin.

The averages which are calculated are $N^{-1}\nu(\theta, N)$, the average fraction of monomer units adsorbed in the solution surface, and $z(\theta, N)$, the mean distance of one end of the chain from the surface when the other end is in the surface. The parameter N is the number of monomer units in the chain, and θ is the energy of adsorption of a monomer unit measured in units of kT. The lattice model and recurrence equations for the associated generalized random walk are described in section 2. The recurrence equations are solved formally in section 3 by the method of generating functions; and formulas for $N^{-1}\nu(\theta, N)$ and $z(\theta, N)$ are obtained in terms of the generating function solution. It is shown in section 4 that there is a critical value of the adsorption energy $\theta_c = \ln(\sqrt{5}-1)$ such that for $\theta > \theta_c$ the molecule exists in an adsorbed state. In particular, for $\theta > \theta_c$ the fraction $N^{-1}\nu(\theta, N)$ is independent of N and greater than zero in the limit $N \to \infty$. The numerical results presented in section 4 for $N^{-1}\nu(\theta, N)$ and $z(\theta, N)$ cover only the adsorbed state of the chain molecule ($\theta > \theta_c$) and apply to the case in which the first two monomer units of one end of the chain lie in the solution surface. There are no qualitative differences between the lattice model investigated in this paper and the simpler lattice models studied in I.

[1] Figures in brackets indicate the literature references at the end of this paper.

2. Lattice Model and Recurrence Equations

We consider a simple-cubic lattice model of the solution-surface system in which the solution surface corresponds to the x-y lattice plane through the point $z=0$. Successive lattice planes through $z=1, 2, \ldots$ represent the solution phase of the system. Polymer chain configurations in the solution correspond to paths generated in a random walk on the lattice between nearest-neighbor sites subject to the restriction that the direction of each step must be at right angles to the direction of the preceding step. The physical presence of the surface is introduced by considering only random walks [3, 4] which never enter the lattice plane through $z=-1$. If a polymer chain is very far from the solution surface, all random walk configurations of a given length are equally likely. However, we are primarily interested in the influence of an adsorbing solution surface on the average conformation of a polymer chain. In our lattice model, all random walk paths of N steps with n steps lying in the surface layer have the same *a priori* probability. Relative to a random walk configuration of N steps with $n-1$ steps lying in the surface, the *a priori* probability of a walk with n steps in the surface layer is greater by the factor e^{θ} where $\theta=\epsilon/kT$ and ϵ is the adsorption energy of a monomer unit.

For convenience, we use a random walk terminology. Consider the problem of computing, for a random walk in which the first two steps lie in the surface layer, the unnormalized or relative probability that at the Nth step the random walker is located at lattice point (m_x, m_y, m_z), where $m_z \geq 0$. There are actually three different relative probabilities $P_x(m_x, m_y, m_z; N+1)$, $P_y(m_x, m_y, m_z; N+1)$, and $P_z(m_x, m_y, m_z; N+1)$ associated with the three different directions from which the random walker arrives at (m_x, m_y, m_z). These three relative probabilities are related to the relative probabilities at the Nth step by the relations

$$P_x(m_x, m_y, m_z; N+1)=(1/4)(E_x^+ + E_x^-)[P_y(m_x, m_y, m_z; N)+P_z(m_x, m_y, m_z; N)],\ m_z \geq 1 \tag{1}$$

$$P_y(m_x, m_y, m_z; N+1)=(1/4)(E_y^+ + E_y^-)[P_x(m_x, m_y, m_z; N)+P_z(m_x, m_y, m_z; N)],\ m_z \geq 1 \tag{2}$$

$$P_z(m_x, m_y, m_z; N+1)=(1/4)(E_z^+ + E_z^-)[P_x(m_x, m_y, m_z; N)+P_y(m_x, m_y, m_z; N)],\ m_z \geq 1 \tag{3}$$

and

$$P_x(m_x, m_y, 0; N+1)=e^{\theta}(1/4)(E_x^+ + E_x^-)[P_y(m_x, m_y, 0; N)+P_z(m_x, m_y, 0; N)] \tag{4}$$

$$P_y(m_x, m_y, 0; N+1)=e^{\theta}(1/4)(E_y^+ + E_y^-)[P_x(m_x, m_y, 0; N)+P_z(m_x, m_y, 0; N)] \tag{5}$$

$$P_z(m_x, m_y, 0; N+1)=e^{\theta}(1/4)E_z^+[P_x(m_x, m_y, 0; N)+P_y(m_x, m_y, 0; N)] \tag{6}$$

where $E_x^{\pm}$ is an operator which is defined by the relation

$$E_x^{\pm}P_j(m_x, m_y, m_z; N)=P_j(m_x \pm 1, m_y, m_z; N). \tag{7}$$

The operators $E_y^{\pm}$ and $E_z^{\pm}$ have similar definitions. Equations (1) to (3) describe the relations between the relative probabilities at the $N+1$th and the Nth steps outside the surface layer. The factor e^{θ} in eqs (4) to (6) accounts for the fact that relative to those configurations where $m_z \geq 1$ at the $N+1$th step, the relative probabilities for those configurations where $m_z=0$ at the $N+1$th step are greater by the factor e^{θ}. The absence of E_z^- in eq (6) is related to the fact that the random walker enters the $z=0$ layer from only one direction.

We are interested in deriving from the solution of eqs (1) to (6) the values of $z(\theta, N)$ the mean distance from the surface at the Nth step and $\nu(\theta, N)$ the mean number of steps in the surface

layer. The definitions of these quantities are

$$\nu(\theta, N) = \left(\frac{d}{d\theta} Q(\theta, N)\right)/Q(\theta, N) = \frac{d}{d\theta} \ln Q(\theta, N) \tag{8}$$

and

$$z(\theta, N) = \sum_{m_x=-\infty}^{\infty} \sum_{m_y=-\infty}^{\infty} \sum_{m_z=0}^{\infty} \sum_{j=1}^{3} m_z P_j(m_x, m_y, m_z; N)/Q(\theta, N) \tag{9}$$

where

$$Q(\theta, N) = \sum_{m_x=-\infty}^{\infty} \sum_{m_y=-\infty}^{\infty} \sum_{m_z=0}^{\infty} \sum_{j=1}^{3} P_j(m_x, m_y, m_z; N) \tag{10}$$

plays the role of a partition function. The subscript $j = 1, 2, 3$ denotes respectively, x, y, and z. It was noted in I and it follows from the structure of the recurrence equations that if one starts a random walk with the first two steps in the surface layer and generates in succession the relative probabilities $P_x(m_x, m_y, m_z; r)$, $P_y(m_x, m_y, m_z; r)$, and $P_z(m_x, m_y, m_z; r)$, these probabilities are linear combinations of exponentials $e^{n\theta}$ where $2 \leq n \leq r+2$. Differentiation of $Q(\theta, N)$ with respect to θ has the effect of generating the sum required for computing the average number n of steps in the surface layer.

It should be noted that the probabilities $P_j(m_x, m_y, m_z; N)$ contain more information than is required to calculate the z component of the mean displacement after N steps and the mean number of steps in the surface layer. In fact, we will not solve eqs (1) to (6). Instead we will proceed as in I and for each value of m_z we will sum the appropriate equations in (1) to (6) over all values of m_x and m_y. The result is

$$p_x(m_z; N+1) = (1/2)[p_y(m_z; N) + p_z(m_z; N)], \quad m_z \geq 1 \tag{11}$$

$$p_y(m_z; N+1) = (1/2)[p_x(m_z; N) + p_z(m_z; N)], \quad m_z \geq 1 \tag{12}$$

$$p_z(m_z; N+1) = (1/4)(E_z^+ + E_z^-)[p_x(m_z; N) + p_y(m_z; N)], \quad m_z \geq 1 \tag{13}$$

and

$$[1-(1-e^{-\theta})]\, p_x(0; N+1) = (1/2)[p_y(0; N) + p_z(0; N)] \tag{14}$$

$$[1-(1-e^{-\theta})]\, p_y(0; N+1) = (1/2)[p_x(0; N) + p_z(0; N)] \tag{15}$$

$$[1-(1-e^{-\theta})]\, p_z(0; N+1) = (1/4)E_z^+[p_x(0; N) + p_y(0; N)] \tag{16}$$

where

$$p_j(m_z; N) = \sum_{m_x=-\infty}^{\infty} \sum_{m_y=-\infty}^{\infty} P(m_x, m_y, m_z; N). \tag{17}$$

We introduce one further transformation in eqs (11) to (16)

$$p(m; N) = p_z(m_z; N) \tag{18}$$

and

$$q(m; N) = (1/2)[p_x(m_z; N) + p_y(m_z; N)]. \tag{19}$$

In terms of these relative probabilities for being in the lattice plane which is m units from the solution surface at the Nth step, we can rewrite eqs (11) to (16) as

$$q(m;\ N+1)=(1/2)[q(m;\ N)+p(m;\ N)],\ m\geq 1 \tag{20}$$

$$p(m;\ N+1)=(1/2)[q(m+1;N)+q(m-1;\ N)],\ m\geq 1 \tag{21}$$

$$[1-(1-e^{-\theta})]q(0;\ N+1)=(1/2)[q(0;\ N)+p(0;\ N)] \tag{22}$$

$$[1-(1-e^{-\theta})]p(0;\ N+1)=(1/2)q(1;\ N). \tag{23}$$

Equations (20) and (22) are obtained by combining (11), (12) and (14), (15), respectively.

The sums in eqs (8) to (10) for $\nu(\theta, N)$ and $z(\theta, N)$, which involve the $P_j(m_x, m_y, m_z; N)$'s, can be replaced by simpler sums involving $p(m; N)$ and $q(m; N)$

$$z(\theta, N)=\sum_{m=0}^{\infty} m[2q(m;\ N)+p(m;\ N)]/Q(\theta, N) \tag{24}$$

and

$$Q(\theta, N)=\sum_{m=0}^{\infty}[2q(m;\ N)+p(m;\ N)]. \tag{25}$$

The starting condition for the random walk, namely, that the first two steps are in the surface layer, corresponds to the statement

$$p(m, 0)=0,\ m\geq 0 \tag{26}$$

and

$$q(0, 0)=e^{2\theta},\ q(m, 0)=0,\ m\geq 1. \tag{27}$$

3. Solution of Recurrence Equations

The recurrence equations (20) to (23) can be solved by introducing generating functions. The procedure used is similar to that used in I. Multiply the equation for $q(m, N+1)$ by $(2\pi)^{-1/2}e^{im\phi}$ and sum over all values of $m\geq 0$. The result is

$$-(1-e^{-\theta})(2\pi)^{1/2}q(0;\ N+1)+\mathcal{Q}(\phi, N+1)=\tfrac{1}{2}\{\mathcal{P}(\phi, N)+\mathcal{Q}(\phi, N)\}, \tag{28}$$

where

$$\mathcal{Q}(\phi, N)=(2\pi)^{-1/2}\sum_{m=0}^{\infty} e^{im\phi}q(m;\ N) \tag{29}$$

and

$$\mathcal{P}(\phi, N)=(2\pi)^{-1/2}\sum_{m=0}^{\infty} e^{im\phi}p(m;\ N). \tag{30}$$

The corresponding equation obtained by combining the equations for the $p(m;\ N+1)$'s is

$$-(1-e^{-\theta})(2\pi)^{-1/2}p(0;\ N+1)+\mathscr{P}(\phi,\ N+1)=\cos\phi\ \mathscr{Q}(\phi,\ N)-\tfrac{1}{2}\ (2\pi)^{-1/2}e^{-i\phi}q(0;\ N). \tag{31}$$

Next multiply eqs (30) and (31) by y^{N+1}, and sum each over all values of N to obtain the pair

$$-(1-e^{-\theta})(2\pi)^{-1/2}[h_0(y)-q(0;\ 0)]+\Lambda(\phi,\ y)-\mathscr{Q}(0,\ 0)=\tfrac{1}{2}\,y[\Gamma(\phi,\ y)+\Lambda(\phi,\ y)] \tag{32}$$

and

$$-(1-e^{-\theta})(2\pi)^{-1/2}[h_0(y)-p(0;\ 0)]+\Gamma(\phi,\ y)-\mathscr{P}(0,\ 0)=y\cos\phi\ \Lambda(\phi,\ y)-\tfrac{1}{2}\ y(2\pi)^{-1/2}e^{-i\phi}k_0(y) \tag{33}$$

where

$$\Lambda(\phi,\ y)=\sum_{N=0}^{\infty}\ y^N\mathscr{Q}(\phi,\ N), \tag{34}$$

$$\Gamma(\phi,\ y)=\sum_{N=0}^{\infty}\ y^N\mathscr{P}(\phi,\ N), \tag{35}$$

$$h_m(y)=\sum_{N=0}^{\infty}\ y^N p(m;\ N), \tag{36}$$

and

$$k_m(y)=\sum_{N=0}^{\infty}\ y^N q(m;\ N). \tag{37}$$

The definitions (29), (30), (36), and (37), when combined with the starting conditions (26) and (27), are substituted in (32) and (33). The result is

$$-\tfrac{1}{2}\ y\Gamma(\phi,\ y)+(1-\tfrac{1}{2}\ y)\Lambda(\phi,\ y)=(2\pi)^{-1/2}[(1-e^{-\theta})k_0(y)+e^{\theta}] \tag{38}$$

and

$$\Gamma(\phi,\ y)-y\cos\phi\Lambda(\phi,\ y)=(2\pi)^{-1/2}[(1-e^{-\theta})h_0(y)-\tfrac{1}{2}\,ye^{-i\phi}k_0(y)]. \tag{39}$$

Next solve eqs (38) and (39) for $\Gamma(\phi,\ y)$ and $\Lambda(\phi,\ y)$ and obtain

$$\Gamma(\phi,\ y)=\frac{(2\pi)^{-1/2}}{1-\frac{1}{2}\,y-\frac{1}{2}\,y^2\cos\phi}\{[(1-e^{-\theta})h_0(y)-\tfrac{1}{2}\ ye^{-i\phi}k_0(y)](1-\tfrac{1}{2}\ y)+[(1-e^{-\theta})k_0(y)+e^{\theta}]y\cos\phi\} \tag{40}$$

$$\Lambda(\phi,\ y)=\frac{(2\pi)^{-1/2}}{1-\frac{1}{2}\ y-\frac{1}{2}\ y^2\cos\phi}\{(1-e^{-\theta})k_0(y)+e^{\theta}+\tfrac{1}{2}\ y[(1-e^{-\theta})h_0(y)-\tfrac{1}{2}\ ye^{-i\phi}k_0(y)]\}. \tag{41}$$

Equations (40) and (41) constitute a pair of implicit equations for the functions $h_0(y)$ and $k_0(y)$ because according to the definitions of $\Gamma(\phi,\ y)$, $\Lambda(\phi,\ y)$, $h_m(y)$, and $k_m(y)$ in (34) to (37) and $\mathscr{P}(\phi,\ N)$ and $\mathscr{Q}(\phi,\ N)$ in (29) and (30)

$$\Gamma(\phi,\ y)=(2\pi)^{-1/2}\sum_{m=0}^{\infty}\ e^{im\phi}h_m(y) \tag{42}$$

and

$$\Lambda(\phi,\ y)=(2\pi)^{-1/2}\ \sum_{m=0}^{\infty} e^{im\phi}k_m(y). \tag{43}$$

A pair of equations for determining $h_0(y)$ and $k_0(y)$ can be obtained by multiplying eqs (40) and (41) by $(2\pi)^{-1/2}$ and integrating with respect to ϕ from $-\pi$ to π

$$h_0(y)=[(1-e^{-\theta})I_0(y)h_0(y)-\tfrac{1}{2}\ yI_1(y)k_0(y)](1-\tfrac{1}{2}\ y)+y[(1-e^{-\theta})k_0(y)+e^{\theta}]I_1(y) \tag{44}$$

and

$$k_0(y)=[(1-e^{-\theta})k_0(y)+e^{\theta}]I_0(y)+\frac{1}{2}\,y(1-e^{-\theta})h_0(y)I_0(y)-\frac{1}{4}\,y^2k_0(y)I_1(y) \tag{45}$$

where

$$I_m(y)=\frac{1}{2\pi}\int_{-\pi}^{\pi}\frac{e^{im\phi}d\phi}{1-\frac{1}{2}\,y-\frac{1}{2}\,y^2\cos\phi}=\left[(1-y)\left(1+\frac{1}{4}\,y^2+\frac{1}{4}\,y^3\right)\right]^{-1/2}$$

$$\times\left\{\frac{1-\frac{1}{2}\,y-\left[(1-y)\left(1+\frac{1}{4}\,y^2+\frac{1}{4}\,y^3\right)\right]^{1/2}}{\frac{1}{2}\,y}\right\}^{|m|} \tag{46}$$

Solving (44) and (45) for $h_0(y)$ and $k_0(y)$, we obtain

$$h_0(y)=\left\{ye^{\theta}I_1(y)\left[1-(1-e^{-\theta})I_0(y)+\frac{1}{4}\,y^2I_1(y)\right]-ye^{\theta}I_0(y)I_1(y)\left[\frac{1}{2}\left(1-\frac{1}{2}\,y\right)-(1-e^{-\theta})\right]\right\}/\mathscr{D}(\theta,\ y) \tag{47}$$

and

$$k_0(y)=\{e^{\theta}I_0(y)[1-(1-\tfrac{1}{2}\,y)(1-e^{-\theta})I_0(y)]+\tfrac{1}{2}\,y^2I_0(y)I_1(y)(e^{\theta}-1)\}/\mathscr{D}(\theta,\ y) \tag{48}$$

where

$$\mathscr{D}(\theta,\ y)=1+(1-e^{-\theta})\left(\frac{1}{2}\,y-2\right)I_0(y)+\frac{1}{4}\,y^2I_1(y)+(1-e^{-\theta})^2I_0(y)\left[I_0(y)\left(1-\frac{1}{2}\,y\right)-\frac{1}{2}\,y^2I_1(y)\right]. \tag{49}$$

Equations (47) to (49) can be simplified with the aid of eq (46) to give

$$h_0(y)=\tfrac{1}{2}\ ye^{\theta}I_1(y)/\mathscr{D}(\theta,\ y) \tag{50}$$

and

$$k_0(y)=I_0(y)/\mathscr{D}(\theta,\ y) \tag{51}$$

where

$$\mathscr{D}(\theta,\ y)=\left[(1-y)\left(1+\frac{1}{4}\,y^2+\frac{1}{4}\,y^3\right)\right]^{-1/2}\left\{\frac{1}{2}\left[(1-y)\left(1+\frac{1}{4}\,y^2+\frac{1}{4}\,y^3\right)\right]^{1/2}-\frac{1}{2}+\frac{1}{4}\,y-\frac{1}{2}\,ye^{-\theta}+e^{-2\theta}\right\}. \tag{52}$$

Substitute the expressions for $h_0(y)$ and $k_0(y)$ obtained in (50) and (51) into eqs (40) and (41) for $\Gamma(\phi, y)$ and $\Lambda(\phi, y)$, and then form the quantity $\Gamma(\phi, y)+2\Lambda(\phi, y)$

$$\Gamma(\phi, y)+2\Lambda(\phi, y)=\frac{(2\pi)^{-1/2}(1+\frac{1}{2}y)}{[1-\frac{1}{2}y-\frac{1}{2}y^2\cos\phi]^{1/2}}\left\{\frac{\frac{1}{2}y(e^{\theta}-1)I_1(y)+I_0(y)\left[-\frac{1}{2}ye^{-i\phi}+2(1-e^{-\theta})\dfrac{2+y\cos\phi}{2+y}\right]}{\mathscr{D}(\theta, y)}\right.$$
$$\left.+2e^{\theta}\frac{2+y\cos\phi}{2+y}\right\}. \tag{53}$$

Equation (53) constitutes an explicit solution of the recurrence equations (20) to (23) which can be used to compute the sums appearing in eqs (24), (25), and (8). In particular, from the definitions of $\Gamma(\phi, y)$ and $\Lambda(\phi, y)$ we have

$$\Gamma(\phi, y)+2\Lambda(\phi, y)=(2\pi)^{-1/2}\sum_{N=0}^{\infty}y^N\sum_{m=0}^{\infty}e^{im\phi}[p(m; N)+2q(m; n)]. \tag{54}$$

If we set $\phi=0$ and select the coefficient of y^N in eq (54) using Cauchy's formula, we obtain an explicit expression for $Q(\theta, N)$

$$Q(\theta, N)=\frac{1}{2\pi i}\oint_{C_0}\frac{dy}{y^{N+1}}(2\pi)^{1/2}[\Gamma(0, y)+2\Lambda(0, y)] \tag{55}$$

where C_0 is a closed contour in the complex y-plane which encloses only the pole of the integrand at $y=0$. Substituting eq (53) in (55) and using eqs (46) and (52), one obtains the explicit formula

$$Q(\theta, N)=\frac{1}{2\pi i}\oint_{C_0}\frac{dy}{y^{N+1}}\frac{1}{1-y}\left\{\frac{\frac{1}{2}y(e^{\theta}-1)I_1(y)+I_0(y)[2(1-e^{-\theta})-\frac{1}{2}y]}{\mathscr{D}(\theta, y)}+2e^{\theta}\right\} \tag{56}$$

or

$$Q(\theta, N)=2e^{\theta}+\frac{1}{2\pi i}\oint_{C_0}\frac{dy}{y^{N+1}}\frac{2}{1-y}$$
$$\times\left\{\frac{(e^{\theta}-1)\left[1-\frac{1}{2}y-\sqrt{(1-y)\left(1+\frac{1}{4}y^2+\frac{1}{4}y^3\right)}\right]y^{-1}+2(1-e^{-\theta})-\frac{1}{2}y}{\sqrt{(1-y)\left(1+\frac{1}{4}y^2+\frac{1}{4}y^3\right)}-1+\frac{1}{2}y-ye^{-\theta}+2e^{-2\theta}}\right\}. \tag{57}$$

The sum $\sum_{m=0}^{\infty}m[p(m; N)+2q(m; N)]$ appearing in eq (24) can be extracted from eq (54)

$$\sum_{m=0}^{\infty}m[p(m; N)+2q(m; N)]=\frac{1}{2\pi i}\oint_{C_0}\frac{dy}{y^{N+1}}\frac{(2\pi)^{1/2}}{i}\frac{d}{d\phi}[\Gamma(\phi, y)+2\Lambda(\phi, y)]\Big|_{\phi=0}. \tag{58}$$

The explicit formula obtained from eq (58) after inserting (53) is

$$\sum_{m=0}^{\infty}m[p(m; N)+2q(m; N)]=\frac{1}{2\pi i}\oint_{C_0}\frac{dy}{y^N}\frac{\frac{1}{2}I_0(y)}{(1-y)\mathscr{D}(\theta, y)} \tag{59}$$

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or

$$\sum_{m=0}^{\infty} m[p(m;\,N)+2q(m;\,N)] = \frac{1}{2\pi i}\oint_{C_0} \frac{dy}{y^N}\frac{1}{1-y}$$

$$\times \left\{\sqrt{(1-y)\left(1+\frac{1}{4}y^2+\frac{1}{4}y^3\right)}-1+\tfrac{1}{2}y-ye^{-\theta}+2e^{-2\theta}\right\}^{-1}. \qquad (60)$$

4. Calculation of $\nu(\theta, N)$ and $z(\theta, N)$ for $N \gg 1$

In this section we evaluate the contour integrals in eqs (57) and (60) for $N \gg 1$ and so obtain expressions for $\nu(\theta, N)$ from eq (8) and $z(\theta, N)$ from eq (24). The procedure which we use to evaluate the contour integrals is similar to that used in I.

Location of singularities. It is first necessary to locate the singularities of the integrands in (57) and (60). In addition to the poles at $y=0$ and $y=1$, there are branch point singularities associated with zeros of the square root function $\sqrt{(1-y)\left(1+\frac{1}{4}y^2+\frac{1}{4}y^3\right)}$, namely, singularities at $y=1$ and at the roots of the cubic equation

$$1+\frac{1}{4}y^2+\frac{1}{4}y^3=0. \qquad (61)$$

It is shown in the appendix that these three roots, y_a, y_b, and y_c, lie outside the unit circle in the complex y-plane. In view of the occurrence of these branch point singularities, we introduce cuts in the complex y-plane as shown in figure 1 in order to define the integrands in eqs (57) and (60) uniquely. The cuts start at the branch points and extend radially outward. The square root function is taken as real and positive on the real axis between $y=0$ and 1. With this definition of the square root function, there may be an additional singularity of the integrands in (57) and (60)

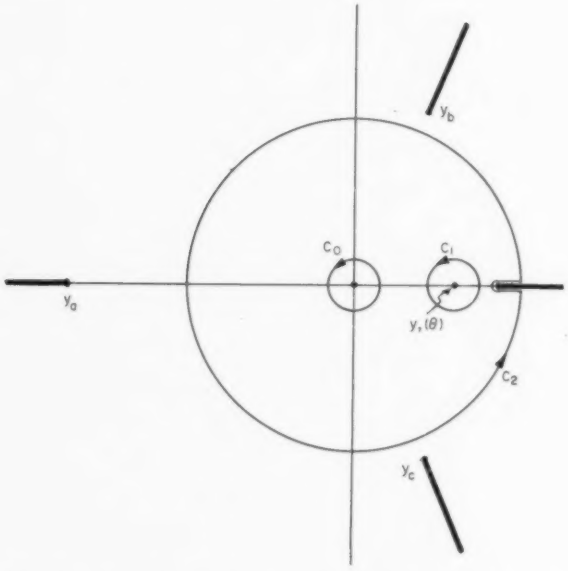

FIGURE 1. *Singularities of integrands, cuts, and contours of integration in the complex y-plane.*

arising from a zero of the denominator

$$g(\theta, y) = \sqrt{(1-y)\left(1+\frac{1}{4}y^2+\frac{1}{4}y^3\right)} - 1 + \frac{1}{2}y + 2e^{-2\theta} - ye^{-\theta}. \tag{62}$$

A numerical investigation of $g(\theta, y)$ for different values of θ shows that there is never more than one root of $g(\theta, y)$ inside the unit circle. When there is a root of $g(\theta, y)$ inside the unit circle, it is real, and it lies between $y=0$ and 1. In order to determine the condition on θ for which there is a real root $y_1(\theta) \leq 1$ of $g(\theta, y)$, consider the plots of the two functions $F(y) = \sqrt{(1-y)\left(1+\frac{1}{4}y^2+\frac{1}{4}y^3\right)}$ and $L(\theta, y) = 1 - 2e^{-2\theta} - (\frac{1}{2} - e^{-\theta})y$ shown in figure 2. The occurrence of the root $y_1(\theta)$ corresponds to an intersection of $F(y)$ and $L(\theta, y)$. For $\theta = \ln 2$, the line $L(\theta, y)$ becomes $L(\ln 2, y) = \frac{1}{2}$. For $\theta > \ln 2$, the slope of $L(\theta, y)$ is negative; and as θ increases the intersection of $L(\theta, y)$ and $F(y)$ moves up toward the point (0, 1), i.e., toward smaller values of $y_1(\theta)$ than $y_1(\ln 2)$. For $\theta < \ln 2$, the slope of $L(\theta, y)$ is positive; and as θ decreases the intersection of $L(\theta, y)$ and $F(\theta, y)$ moves down toward the point (1, 0). The critical value of θ, for which the intersection of $L(\theta, y)$ and $F(y)$ occurs at (1, 0) can be determined by solving the equation $g(\theta, 1) = 0$, i.e.,

$$-1 + \tfrac{1}{2} + 2e^{-2\theta} - e^{-\theta} = 0. \tag{63}$$

The value of θ at which $y_1(\theta) = 1$ is

$$\theta_c = \ln(\sqrt{5} - 1). \tag{64}$$

There are no other singularities of the integrands in (57) and (60).

Deformation of the contour of integration. Having determined the positions and types of singularities of the integrands in the integral representations of $Q(\theta, N)$ and $\sum_{m=0}^{\infty} m[p(m; N) + 2q(m; N)]$, we will now evaluate these integrals in the limit in which N is large and $\theta > \theta_c$. As in I, the details of the calculation are different, depending upon whether $\theta > \theta_c$, $\theta < \theta_c$, or $\theta = \theta_c$.

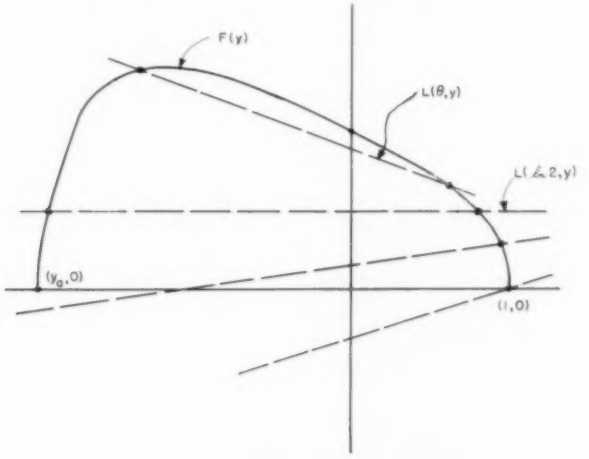

FIGURE 2. *Plots of* $F(y) = \left[(1-y)\left(1+\frac{1}{4}y^2+\frac{1}{4}y^3\right)\right]^{1/2}$ *and* $L(\theta, y) = 1 - 2e^{-2\theta} - \left(\frac{1}{2} - e^{-\theta}\right)y$ *versus* y *for real* y, $0 \leq y \leq 1$.

The results in each case are qualitatively the same as in I. Therefore, we will limit our discussion to the case $\theta > \theta_c$.

Consider the integral

$$\mathcal{I} = \frac{1}{2\pi i} \oint \frac{f(y)}{g(\theta, y)} \frac{dy}{y^{N+1}} \tag{65}$$

around the three contours C_0, C_1, and C_2 shown in figure 1. Denote these integrals by $\mathcal{I}_0$, $\mathcal{I}_1$, and $\mathcal{I}_2$, respectively. Suppose that the integrand $f(y)/g(\theta, y)y^{N+1}$ is the integrand in eq (57) or (60) so that $\mathcal{I}_0 = Q(\theta, N)$ or $\mathcal{I}_0 = \sum_{m=0}^{\infty} m[p(m; N) + 2q(m; N)]$, respectively. The contour C_1 encloses $y_1(\theta)$, and the contour C_2 consists of a circular part whose radius is $1+\delta$, and an indented part around the branch point at $y = 1$. With these definitions, the integrals satisfy the relation

$$\mathcal{I}_0 = \mathcal{I}_2 - \mathcal{I}_1 \tag{66}$$

We first evaluate $\mathcal{I}_1$ and indicate why $\mathcal{I}_2$ is negligible compared to $\mathcal{I}_1$ for $N >> 1$. The value of $\mathcal{I}_1$ is simply the residue [5] at $y_1 = y_1(\theta)$

$$\mathcal{I}_1 = f(y_1)/g'(\theta, y_1)y_1^{N+1} \tag{67}$$

where $g'(\theta, y_1)$ denotes $\frac{d}{dy} g(\theta, y)|_{y=y_1}$. Thus $\mathcal{I}_1$ is proportional to the $(N+1)^{st}$ power of a number which is larger than one. As in I, it can be verified in the case of the contour integral $\mathcal{I}_2$ that the contribution from the circular part of the contour is proportional to $(1+\delta)^{-N}$, and that the contribution from the remaining part of the contour is small compared to $\left(\frac{1}{y_1}\right)^{N+1}$. Therefore, in the limit $N \gg 1$, we can neglect $\mathcal{I}_2$ compared to $\mathcal{I}_1$ and write eq (66) as

$$\mathcal{I}_0 \doteq -\mathcal{I}_1 \tag{68}$$

This approximation is excellent for large finite values of N provided that θ is not too close to θ_c, i.e., provided that y_1 is not too close to the branch point $y = 1$. Having established the relations (67) and (68) for both integrals (57) and (60), we can now calculate the values of $\nu(\theta, N)$ and $z(\theta, N)$. First we have from eq (8)

$$\nu(\theta, N) = \frac{\partial}{\partial \theta} \ln Q(\theta, N) \doteq -N \frac{\partial y_1}{\partial \theta} \Big/ y_1. \tag{69}$$

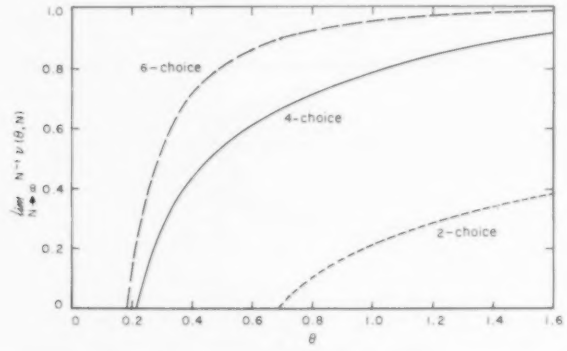

FIGURE 3. *Average fraction of adsorbed monomer units* $N^{-1}\nu(\theta, N)$ *versus adsorption energy* θ *(solid curve) for* $\theta > \theta_c$.
For comparison, the corresponding curves for the 6-choice simple cubic lattice (dashed curve) and the 2-choice simple cubic (dotted curve) are included, from reference I.

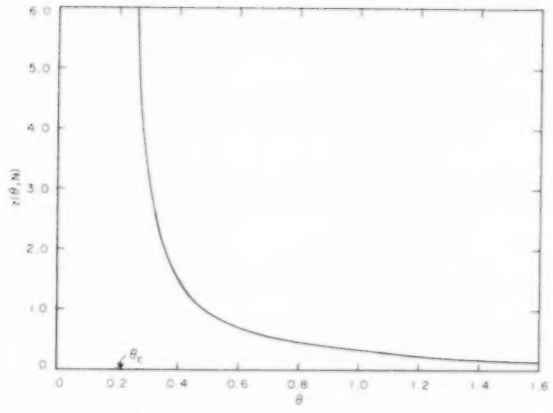

FIGURE 4. *Mean distance of end of polymer chain from surface* $z(\theta, N)$ *versus adsorption energy* θ *for* $\theta > \theta_c$.

In eq (69), we have dropped terms which are not proportional to N. It is seen that the result obtained here for the case of the 4-choice s.c. lattice when $\theta > \theta_c$ is similar to the result obtained in I, namely, on the average a finite fraction of all steps are adsorbed in the surface for $N \gg 1$. In the case of eq (24) we have

$$z(\theta, N) \doteq \frac{1}{2} y_1 \left\{ (e^{\theta} - 1)\left[1 - \frac{1}{2} y_1 - \sqrt{(1 - y_1)\left(1 + \frac{1}{4} y_1^2 + \frac{1}{4} y_1^3 \right)} \right] y_1^{-1} + 2(1 - e^{-\theta}) - \frac{1}{2} y_1 \right\}^{-1}, \tag{70}$$

a result which is independent of N for $N \gg 1$.

The values of $N^{-1}\nu(\theta, N)$ and $z(\theta, N)$ in eqs (69) and (70) have been determined numerically by F. McCrackin; and the results are presented graphically in figures 3 and 4 for $\theta > \theta_c$. Values of $N^{-1}\nu(\theta, N)$ obtained in I for the 6-choice simple cubic lattice and the 2-choice simple cubic lattice are also included in figure 3 for comparison. Although results have only been presented for adsorption energies greater than θ_c, examination of the behavior of the integrands in (57) and (60) for $\theta < \theta_c$ and $\theta = \theta_c$ in the neighborhood of $y = 1$ shows that the results for the 4-choice simple cubic lattice are qualitatively similar to the results for the lattices studied in I over the entire range of values of θ.

I thank F. McCrackin for calculating the numerical values of $N^{-1}\nu(\theta, N)$ and $z(\theta, N)$.

5. Appendix

The roots of the cubic equation

$$\frac{1}{4} y^3 + \frac{1}{4} y^2 + 1 = 0 \tag{A1}$$

are the reciprocals of the roots of the equation

$$z^3 + \frac{1}{4} z + \frac{1}{4} = 0.$$

Therefore the roots of (A1) are

$$y_a = -2\{[(1+1/27)^{1/2}+1]^{1/3}-[(1+1/27)^{1/2}-1]^{1/3}\}^{-1}$$

$$\cong -1.968$$

$$y_b = 4\{[(1+1/27)^{1/2}+1]^{1/3}-[(1+1/27)^{1/2}-1]^{1/3}-i\sqrt{3}([(1+1/27)^{1/2}+1]^{1/3}+[(1+1/27)^{1/2}-1]^{1/3})\}^{-1}$$

$$\cong 0.497+1.308i$$

$$y_c \cong 0.497-1.308i$$

Thus all three roots, y_a, y_b, and y_c, lie outside the unit circle.

6. References

[1] R. J. Rubin, J. Chem. Phys. **43,** 2392 (1965). This paper will be referred to as I. There is a large body of literature, much of it recent, concerned with this problem. The reader is referred to I, and references [1–4] therein for additional references.

[2] F. McCrackin, Bull. Am. Phys. Soc. **10,** 380 (1965), to be published in J. Chem. Phys.

[3] A. Silberberg, J. Phys. Chem. **66,** 1872 (1962).

[4] E. A. DiMarzio, J. Chem. Phys. **42,** 2101 (1965).

[5] E. T. Whittaker and G. N. Watson, A Course of Modern Analysis (University Press, Cambridge, 1947).

(Paper 69B4–159)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 69B, No. 4, October–December 1965

Groups of Unimodular Circulants

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(August 12, 1965)

A method to determine a basis of the group of rational integral symmetric positive definite unimodular $n \times n$ circulants for any n, is presented. This method uses the correspondence between unimodular circulants and units of the algebraic number field $R(\zeta)$, where ζ is a primitive nth root of unity. Known results are used to obtain generators of certain aperiodic subgroups of the abelian, finitely generated group of units in $R(\zeta)$. The correspondence, then, produces the desired basis elements. The number of basis elements for each n is proved to be $\left[\frac{n}{2}\right]+1-\sigma_0(n)$, where $\sigma_0(n)$ is the number of positive divisors of n. In addition, an upper bound for the number of congruence classes of these circulants is obtained, where congruence is relative to rational symmetric unimodular $n \times n$ circulants.

Key Words: Algebraic numbers, circulant matrices, abelian groups.

In 1956, M. Newman and O. Taussky [7][1] exhibited a rational integral symmetric positive definite unimodular 8×8 circulant that was not of the form AA', where A is a rational integral 8×8 circulant and A' its transpose. The method they used in obtaining the positive definite circulant can be adapted to find generators of groups of rational integral symmetric positive definite unimodular circulants for particular values of n. However, difficult problems arise when the method is applied for arbitrary n.

This paper presents an alternate method of determining generators of these groups through the use of a correspondence, investigated by O. Taussky [8], between units of the algebraic number field $R(\zeta)$, where ζ is a primitive nth root of unity, and unimodular circulants. The group of units in $R(\zeta)$ is abelian and finitely generated. By restricting the discussion to certain aperiodic subgroups of this group, results conveniently compiled in Hecke [2, pp 38–44] can be used to determine generators of the subgroups. By the correspondence, then, generators of groups of rational integral symmetric positive definite unimodular $n \times n$ circulants are obtained. In addition, the number of these generators is proved to be $\left[\frac{n}{2}\right]+1-\sigma_0(n)$, where $\sigma_0(n)$ is the number of positive divisors of n. Furthermore, an upper bound for the number of classes of these circulants is obtained for arbitrary n, where two of these circulants A and B are in the same class if and only if there is a rational symmetric unimodular $n \times n$ circulant S such that $A = S'BS$.

[1] Figures in brackets indicate the literature references at the end of this paper.

First, the notation used throughout this paper will be established. Let P be the $n \times n$ permutation matrix

$$\begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ & \dots & & & \\ 1 & 0 & 0 & \dots & 0 \end{pmatrix}$$

Then P is a full cycle. Since P is normal there exists a unitary matrix U such that $U^* P U = D_p$, where D_p is a diagonal matrix and U^* is the conjugate transpose of U. Assume ζ is a primitive nth root of unity. Then U may be taken as $\frac{1}{\sqrt{n}}(\zeta^{ij})$ for $1 \leq i, j \leq n$. It follows that $D_p = \operatorname{diag}(\zeta, \zeta^2, \dots, \zeta^n)$ and the eigenvalues of P are the nth roots of unity.

Let C be an $n \times n$ rational integral unimodular circulant given by $C = a_0 I + a_1 P + \dots + a_{n-1} P^{n-1}$. Denote by G the group of all such circulants; G_1, the subgroup of symmetric elements of G; and G_2, the subgroup of positive definite elements of G_1. We will prove that G is a finitely generated abelian group (Theorem 1). The subgroup G_1 and G_2 of G, then, are also finitely generated and abelian. It follows that each of the groups G, G_1, G_2 can be decomposed into the direct product of a periodic group and an aperiodic group [9, p. 91]. Let R be the field of rationals and denote by E the finitely generated multiplicative abelian group of units in $R(\zeta)$; E_1, the subgroup of real elements of E; and E_2, the subgroup of totally positive elements of E_1.

That is, E_2 consists of those elements of E_1 which are positive together with all their conjugates. (The notation and definitions of all groups in this paper are given in the appendix.)

With the above notation, Dirichlet's Theorem [2, p. 124] can be stated as follows:

If the defining polynomial of $R(\zeta)$ is $p(x)$, and if among the roots of $p(x)$ there are r_1 real and $2r_2$ imaginary ones, then the number of elements of infinite order in the basis of E is $r = r_1 + r_2 - 1$. There exist $r+1$ units $\zeta, \eta_1, \ldots, \eta_r$, where ζ is a primitive wth root of unity, such that any element ϵ of E has a unique representation $\epsilon = \zeta^{a_0}\eta_1^{a_1} \ldots \eta_r^{a_r}$, where a_i are rational integers for $1 \leq i \leq r$ and a_0 is a rational integer modulo w.

Note that the basis elements $\eta_1, \ldots, \eta_r$ of infinite order can be taken to be real [1, p. 185].

Each group E, E_1, and E_2 can also be decomposed into a direct product of a periodic group and an aperiodic group. Let E_1' be the largest aperiodic subgroup of E_1. Define H, H_1, and H_2 as follows: H is the largest aperiodic subgroup of G; H_1 is the subset of elements of H all of whose eigenvalues belong to E_1'; and $H_2 = H_1 \cap G_2$.

The following theorem will be of importance. A sketch of the proof was published as part of a paper by M. Newman [6]; the proof was suggested by O. Taussky. The proof is included here because some of the details in the proof will be used in later proofs.

THEOREM 1. *G is a finitely generated abelian group with respect to matrix multiplication.*

PROOF. It is clear that G is an abelian group with respect to matrix multiplication. To show that G is finitely generated, we embed it in a finitely generated group. Let $C = a_0 I + a_1 P + \ldots + a_{n-1}P^{n-1} = \epsilon(P)$ be an arbitrary element of G. Since $P = UD_pU^*$, then $C = UD_cU^*$, where $D_c = \operatorname{diag}(\epsilon(\zeta), \ldots, \epsilon(\zeta^n))$ and U is the unitary matrix mentioned earlier. But D_c can be written as a product in the following way:

$$D_c = \operatorname{diag}(\epsilon(\zeta), 1, \ldots, 1)\operatorname{diag}(1, \epsilon(\zeta^2), 1, \ldots, 1)\ldots \operatorname{diag}(1, \ldots, \epsilon(\zeta^n))$$

where $\epsilon(\zeta^j) \in E$ for $1 \leq j \leq n$ (since $\det D_c = \det C = \pm 1$).

With the notation in the above statement of Dirichlet's Theorem, each unit $\epsilon(\zeta^j)$, $1 \leq j \leq n$, has the following unique representation:

$$\epsilon(\zeta^j) = \zeta^{a_{0j}}\eta_1^{a_{1j}}\eta_2^{a_{2j}} \ldots \eta_r^{a_{rj}}.$$

Then

$$\operatorname{diag}(1, \ldots, 1, \epsilon(\zeta^j), 1, \ldots, 1) = \operatorname{diag}(1, \ldots, 1, \zeta^{a_{0j}}, 1, \ldots, 1) \prod_{i=1}^{r} \operatorname{diag}(1, \ldots, 1, \eta_i^{a_{ij}}, 1, \ldots, 1),$$

where the elements $\epsilon(\zeta^j)$, $\zeta^{a_{0j}}$, $\eta_i^{a_{ij}}$ appear in the jth position on the diagonal for $1 \leq j \leq n$. Let

$$A_{0j} = U \operatorname{diag}(1, \ldots, 1, \zeta, 1, \ldots, 1)\, U^*$$

$$A_{ij} = U \operatorname{diag}(1, \ldots, 1, \eta_i, \ldots, 1)\, U^*,$$

$1 \leq i \leq r$, $1 \leq j \leq n$ (i.e., the elements ζ and η_i appear in the jth position on the diagonal of A_{ij}, $1 \leq j \leq n$). Then there are finitely many matrices of the form A_{ij} such that

$$C = \prod_{\substack{i=0,1,\ldots,r \\ j=1,\ldots,n}} A_{ij}^{a_{ij}}.$$

However, the matrices A_{ij} need not be circulants.

Consider the group Γ generated by the A_{ij}'s defined above for $0 \leq i \leq r$ and $1 \leq j \leq n$. It is clear that Γ is finitely generated. Furthermore, Γ is abelian because diagonal matrices commute. Thus Γ is a finitely generated abelian group which contains G as a subgroup and the theorem is proved.

COROLLARY 1. All eigenvalues of an element of $G(G_i, i = 1, 2)$ are elements of $E(E_i, i = 1, 2)$.

A relationship between G and a certain group of units will be established for which the following properties of units in E are needed.

LEMMA 1. *Let $\Phi_n(x)$ be the cyclotomic polynomial of degree $\varphi(n)$ and let ν be a primitive n^{th} root of unity. Then the sum of the coefficients of a unit $q(\nu) \in E$ can be changed modulo $\Phi_n(1)$ without changing the unit.*

PROOF. Let $q(x)$ be an integral polynomial such that $q(\nu)$ is a unit in E. Define a polynomial $q_t(x)$ as follows: $q_t(x) = q(x) + t\Phi_n(x)$, where t is an integer. Then $q_t(\nu) = q(\nu)$ and $q_t(1) = q(1) + t\Phi_n(1)$. Since $q(1)$ is the sum of the coefficients of $q(\nu)$ the lemma is proved.

LEMMA 2. $\Phi_n(1) = \begin{cases} p \text{ if } n = p^\alpha \\ 1 \text{ otherwise,} \end{cases}$ *where p is a prime and α is a positive integer.* [5, p. 160]

PROOF. Let $\mu(d)$ be the Möbius function and let ζ be a primitive nth root of unity. Then

$$\Phi_n(x) = \prod_{(r,\, n)=1} (x - \zeta^r) = \prod_{d|n} (x^{n/d} - 1)^{\mu(d)} = \prod_{d|n} \left(\frac{x^{n/d} - 1}{x - 1}\right)^{\mu(d)}, \quad n > 1.$$

The last equality follows because

$$\prod_{d|n} (x-1)^{\mu(d)} = (x-1)^{\sigma} = 1 \text{ for } n > 1 \text{ and } \sigma = \sum_{d|n} \mu(d).$$

Thus, for $n > 1$

$$\Phi_n(1) = \prod_{(r,\, n)=1} (1 - \zeta^r) = \prod_{d|n} \left(\frac{n}{d}\right)^{\mu(d)} = \prod_{d|n} d^{-\mu(d)} = \begin{cases} p \text{ if } n = p^\alpha \\ 1 \text{ otherwise.} \end{cases}$$

From Lemma 1 it follows that the representation of a unit $q(\nu)$ in E can be uniquely given either by specifying $q(\eta)$ for some nonprimitive nth root of unity (for example, $\eta = 1$) or by specifying the polynomial $q(x)$.

EXAMPLE. A primitive 5th root of unity ν satisfies the relation $\nu^4 + \nu^3 + \nu^2 + \nu + 1 = 0$. Consider the distinct polynomials $q_1(x) = 1 - x - x^4$ and $q_2(x) = 2 + x^2 + x^3$. Then

$$q_1(\nu) = 1 - \nu - \nu^4 = 2 + \nu^2 + \nu^3 = q_2(\nu)$$

$$q_1(\nu^2) = 1 - \nu^2 - \nu^3 = 2 + \nu + \nu^4 = q_2(\nu^2)$$

$$q_1(\nu^3) = q_1(\nu^2) = q_2(\nu^3)$$

$$q_1(\nu^4) = q_1(\nu) = q_2(\nu^4)$$

$$q_1(\nu^5) = q_1(1) = -1,\ q_2(\nu^5) = q_2(1) = 4.$$

Let $\epsilon(x) = a_0 + a_1 x + \ldots + a_{n-1}x^{n-1}$ be the integral polynomial such that $\epsilon(\zeta^k)$, $1 \leq k \leq n$, are eigenvalues of the circulant $\epsilon(P)$ in G. (Let $\zeta = \exp \frac{2\pi i}{n}$ for definiteness.) From the proof of Theorem 1 it follows that these eigenvalues have a fixed ordering and, since their representation is fixed by $\epsilon(x)$, uniquely determine $\epsilon(P)$. These eigenvalues occur precisely once among the numbers $\epsilon(\zeta^{r\,n/d})$, where d runs over the positive divisors of n, and r runs over those integers such that $1 \leq r \leq d$, $(r, d) = 1$. Denote the divisors, including 1 and n, by $d_1, \ldots, d_m$, where $1 = d_1 < d_2 < \ldots < d_m = n$ and $m = \sigma_0(n)$.

Corresponding to each $\epsilon(x)$ as defined above there is an m-tuple $(\epsilon(\zeta^{d_1}), \ldots, \epsilon(\zeta^{d_m}))$ of units of E. (When n is a prime p, for example, $d_1 = 1$, $d_2 = d_m = p$ and the m-tuples have the form $(\epsilon(\zeta), \epsilon(1))$.) Let $\mathscr{F}$ be the set of all such m-tuples. Define the mapping θ of G into $\mathscr{F}$ by

$$\theta\colon \epsilon(P) \longrightarrow (\epsilon(\zeta^{d_1}), \ldots, \epsilon(\zeta^{d_m}))$$

and multiplication of elements of $\mathscr{F}$ by

$$(\epsilon(\zeta^{d_1}), \ldots, \epsilon(\zeta^{d_m})) \cdot (\delta(\zeta^{d_1}), \ldots, \delta(\zeta^{d_m}))$$

$$= (\epsilon(\zeta^{d_1}) \cdot \delta(\zeta^{d_1}), \ldots, \epsilon(\zeta^{d_m}) \cdot \delta(\zeta^{d_m})).$$

THEOREM 2. *θ is an isomorphism of G onto $\mathscr{F}$.*

PROOF. The mapping θ is onto. Let $\epsilon(x)$ be an integral polynomial such that $\epsilon(\zeta^d) \epsilon E$ for each $d|n$ and define $\Lambda_d = \operatorname{diag}(\zeta^{r_1 n/d}, \ldots, \zeta^{r_k n/d})$, where $k = \varphi(d)$ and $1 = r_1 < r_2 < \ldots < r_k \leq d$ are the numbers relatively prime to d. (That is, the diagonal elements of Λ_d are the primitive dth roots of unity.) Form the direct sum $\sum_{d|n}^{*} \Lambda_d$. For a suitable permutation matrix Q,

$$Q \sum_{d|n}^{*} \Lambda_d Q' = \operatorname{diag}(\zeta, \ldots, \zeta^n) = D_\epsilon.$$

Also

$$\epsilon(\Lambda_d) = \operatorname{diag}(\epsilon(\zeta^{r_1 n/d}), \ldots, \epsilon(\zeta^{r_k n/d}))$$

so that

$$Q\left(\sum_{d|n}^{*} \epsilon(\Lambda_d)\right) Q' = \operatorname{diag}(\epsilon(\zeta), \ldots, \epsilon(\zeta^n)) = D_\epsilon$$

and

$$UQ\left(\sum_{d|n}^{*} \epsilon(\Lambda_d)\right) Q'U^* = \epsilon(P) \epsilon G.$$

The mapping θ is 1–1. Let $\epsilon_1(P)$ and $\epsilon_2(P)$ be elements of G such that the m-tuples $\theta(\epsilon_1(P))$ and $\theta(\epsilon_2(P))$ are identical elements of $\mathscr{F}$. Then $\epsilon_1(P)$ and $\epsilon_2(P)$ have the same eigenvalues ordered in the same way, hence $\epsilon_1(P) = \epsilon_2(P)$.

Finally, if $\epsilon(P)$ and $\delta(P)$ are any two elements in G, then $\theta(\epsilon(P)) \cdot \theta(\delta(P)) = (\epsilon(\zeta^{d_1}), \ldots, \epsilon(\zeta^{d_m})) \cdot (\delta(\zeta^{d_1}), \ldots, \delta(\zeta^{d_m})) = (\epsilon(\zeta^{d_1}) \cdot \delta(\zeta^{d_1}), \ldots, \epsilon(\zeta^{d_m}) \cdot \delta(\zeta^{d_m})) = \theta(\epsilon(P) \cdot \delta(P))$, hence θ preserves multiplication.

COROLLARY 2. *If $\delta(P) \epsilon G_i$, $i = 1, 2$, then $\theta(\epsilon(P))$ is an m-tuple of elements of E_i, $i = 1, 2$.*

PROOF. Assume $\epsilon(P) \epsilon G_1$. Then $\epsilon(P) = \epsilon(P)^* = UD_\epsilon^* U^* = UD_\epsilon U^*$ so that $D_\epsilon = D_\epsilon^*$, which implies $\epsilon(\zeta^k)$, $1 \leq k \leq n$, is real.

Assume $\epsilon(P) \epsilon G_2$. Then $D_\epsilon = D_\epsilon^*$ and D_ϵ is positive definite, hence $\epsilon(\zeta^k) \epsilon E_2$, $1 \leq k \leq n$.

In order that the results on aperiodic groups [2, pp. 38–44] can be used it is necessary to consider the restriction of θ to an aperiodic subgroup H_1 of G defined as follows: H_1 is the set of elements of G_1 all of whose eigenvalues belong to the largest aperiodic subgroup E_1' of E_1.

THEOREM 3. *If $n \neq p^\alpha$, where p is a prime and α is a positive integer, then θ maps H_1 onto the subset F_1 of $\mathscr{F}$ consisting of m-tuples $(\epsilon(\zeta^{d_1}), \ldots, \epsilon(\zeta^{d_m}))$ of elements of E_1'. If $n = p^\alpha$, then θ maps H_1 onto a subset F_1' of F_1, where F_1' consists of m-tuples of elements of a subgroup E_1'' of E_1 defined as follows:*

$$E_1'' = \{\epsilon(\zeta) \epsilon E_1' \mid \epsilon(1) \equiv 1 \pmod{p}\},$$

where $\epsilon(x)$ is an integral polynomial such that $\epsilon(P)$ is a circulant in H_1 with eigenvalues $\epsilon(\zeta^k)$, $1 \leq k \leq n$.

PROOF. It follows from Corollary 2 that the units in the m-tuples of F_1 are real. Also, $\epsilon(\zeta^n) = \epsilon(1) = 1$ since $\epsilon(\zeta^n)$ is a real eigenvalue of a unimodular matrix with integral coefficients and an element of an aperiodic group. By Lemma 1, any polynomial $\epsilon_t(x)$ of the form $\epsilon_t(x) = \epsilon(x) + t\Phi_n(x)$ and such that $\epsilon_t(P)$ is a circulant in H_1 has coefficient sum $\epsilon_t(1) \equiv (1) \pmod{\Phi_n(1)}$. The theorem follows from Lemma 2.

Theorems related to the number of basis elements of the aforementioned groups will now be established.

THEOREM 4. *If $n = p^\alpha$, then $(F_1 : F_1') = p - 1$.*

PROOF. Let k be an odd primitive root modulo p

and define the function $\mu_{2k}(x)$ as follows:

$$\mu_{2k}(x)=\begin{cases}\dfrac{1-x^k}{1-x}\cdot\dfrac{1-x^{-k}}{1-x^{-1}}=x^{1-k}\left(\dfrac{1-x^k}{1-x}\right)^2, & x\neq 1\\ (1+x+\cdots+x^{k-1})^2, & x=1.\end{cases}$$

Then $\mu_{2k}(\zeta)\epsilon E_1$, where ζ is a primitive p^ath root of unity. Let $\mu_k(x)$ be the positive square root of $\mu_{2k}(x)$. Then

$$\mu_k(\nu)=\nu^{\frac{1-k}{2}}\cdot\frac{1-\nu^k}{1-\nu}\epsilon E_1', \text{ for } \nu=\zeta, \zeta^p, \ldots, \zeta^{p^{a-1}},$$

and $\mu_k(1)=k$, hence $\mu_k(1)^r=k^r$.

Now, let $q(x)$ be an integral polynomial such that $(q(\zeta), q(\zeta^p), \ldots, q(\zeta^{p^a}))\epsilon F_1$. Then $(q(1), p)=1$. For, if $(q(1), p)=p$, then $q(1)=c\cdot p$ for some integer c. Consider the polynomial $g(x)=q(x)-c\Phi_{p^a}(x)$. Since $g(1)=0$, $(x-1)|g(x)$ and $q(x)=c\Phi_{p^a}(x)+r(x)(x-1)$, where $r(x)$ is a polynomial with rational integral coefficients. Then $q(\zeta)=r(\zeta)(\zeta-1)$ so that $\pm 1=\Pi q(\zeta)=\Pi r(\zeta)(\zeta-1)=p\Pi r(\zeta)$ where the products are taken over all primitive p^ath roots of unity. But this implies $p|1$ which is a contradiction. Thus $(q(1), p)=1$ and there exists an r, $1\leq r\leq p-1$, such that $q(1)\mu_k(1)^r\equiv 1 \pmod p$. Thus $q(\nu)\cdot\mu_k(\nu)^r\epsilon E_1''$, for this value of r and for $\nu=\zeta, \zeta^p, \ldots, \zeta^{p^a}$, hence $(F_1:F_1')\leq p-1$.

From the above result it follows that F_1 can be written as a set theoretic sum with at most $p-1$ summands of the form $\mu_k^i\cdot F_1'$, where μ_k^i is defined as $\mu_k^i=(\mu_k(\zeta)^i, \ldots, \mu_k(\zeta^{p^a})^i)\epsilon F_1$ for $0\leq i\leq p-2$. But there must be at least $p-1$ summands. Assume $F_1=\sum_{i=0}^{p-2}\mu_k^i\cdot F_1'$ and $\mu_k^t\cdot F_1'=\mu_k^s\cdot F_1'$, where $0\leq t, s\leq p-2$. Then $\mu_k^t\cdot\mu_k^{-s}\epsilon F_1'$ and $\mu_k(1)^t\cdot\mu_k(1)^{-s}=k^{t-s}\equiv 1 \pmod p$. This implies $(p-1)|(r-s)$, hence $r=s$ and $(F_1:F_1')\geq p-1$ which proves the theorem.

NOTE. Let $F=\theta(H)$. Then it is also true that $(F:F_1')=p-1$ since the basis elements of the group E can be chosen to be real.

The following theorem is one of the principal results in this paper.

THEOREM 5. *The number* b(n) *of basis elements of the largest aperiodic subgroup* H *of* G *is given by*

$$\mathrm{b(n)}=\sum_{\substack{d\mid n\\ d>2}}\left(\tfrac{1}{2}\,\varphi(\mathrm{d})-1\right)=\left[\frac{\mathrm{n}}{2}\right]+1-\sigma_0(\mathrm{n}),$$

where σ_0(n) *is the number of positive divisors of* n.

PROOF. Let $\epsilon(x)$ be an integral polynomial such that $\epsilon(P)\epsilon H$ has eigenvalues $\epsilon(\zeta), \ldots, \epsilon(\zeta^n)$ in E. Denote the image of H under the mapping θ by F. Then F is an aperiodic subgroup of $\mathcal{F}$ consisting of m-tuples of the form

$$(\epsilon(\zeta^{d_1}), \ldots, \epsilon(\zeta^{d_m}))=\prod_{j=1}^{m}(1, \ldots, 1, \epsilon(\zeta^{d_j}), 1, \ldots, 1),$$

where $d_1, \ldots, d_m$ are the positive divisors of n. (Note that ζ^{d_i} is a primitive $\frac{n}{d_i}$th root of unity, $1\leq i\leq m$, and that both $\frac{n}{d_i}$ and d_i run through all positive divisors of n.)

Let $d>2$ be a divisor of n. The defining polynomial of a primitive dth root of unity ν is $\Phi_d(x)$. This polynomial has $\varphi(d)$ complex roots and no real ones. By Dirichlet's theorem there are $\frac{1}{2}\varphi(d)-1$ basis elements of infinite order in the group of units in $R(\nu)$. (The group is trivial when $d=1$ or 2.) A basis of the aperiodic group F, then, consists of $\Sigma(\frac{1}{2}\varphi(d)-1)$ elements, where the summation is over all positive divisors d of n greater than 2, and the first equality is proved.

The second equality can be proved by considering two cases.

(i) n is odd. Then

$$\sum(\tfrac{1}{2}\varphi(d)-1)=\tfrac{1}{2}\sum\varphi(d)-(\sigma_0(n)-1)=\tfrac{1}{2}(n-1)\sigma_0(n)+1=\left[\frac{n}{2}\right]+1-\sigma_0(n).$$

(ii) n is even. Then

$$\sum(\tfrac{1}{2}\varphi(d)-1)=\tfrac{1}{2}\sum\varphi(d)-(\sigma_0(n)-2)=\tfrac{1}{2}(n-2)-\sigma_0(n)+2=\left[\frac{n}{2}\right]+1-\sigma_0(n).$$

By a direct application of Theorem 5 it follows that $b(p)=\dfrac{p-3}{2}$, where p is a prime greater than 2, and that $b(2p)=2\cdot b(p)=p-3$. More generally, if n is odd, then $b(2n)=2\cdot b(n)$.

The following table gives the values of $b(n)$ for $1\leq n\leq 16$.

n	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
$b(n)$	0	0	0	0	1	0	2	1	2	2	4	1	5	4	4	4

Assume $f_1, \ldots, f_r$ is a basis of F. That is, f_i, $1\leq i\leq n$, is an m-tuple of units of E as defined above. Then bases for $F_1(F_1')$ and $F_2=\theta(H_2)$ of the following form can be found [2]:

$$f_1^{(1)}=f_1^{k_{11}}\quad f_2^{k_{12}}\cdots f_r^{k_{1r}}$$
$$f_2^{(1)}=\quad f_2^{k_{22}}\cdots f_r^{k_{2r}}$$
$$f_r^{(1)}=\quad f_r^{k_{rr}}$$

and

$$f_1^{(2)}=f_1^{(1)^{k_{11}}}\quad f_2^{(1)^{k_{12}}}\cdots f_r^{(1)^{k_{1r}}}$$
$$f_2^{(2)}=\quad f_2^{(1)^{k_{22}}}\cdots f_r^{(1)^{k_{2r}}}$$
$$f_r^{(2)}=\quad f_r^{(1)^{k_{rr}}},$$

respectively, where $|k_{11}k_{22} \cdots k_{rr}| = (F:F_1)$ or $(F:F_1')$ and $|1_{11}1_{22} \cdots 1_{rr}| = (F_1:F_2)$ or $(F_1':F_2)$. These bases are not necessarily unique but when one is known it is possible to determine bases for H, H_1, and H_2 by the correspondence in Theorem 2. Then $r = b(n)$. Furthermore it will be shown in Theorem 8 that an upper bound for the value of $|1_{11}1_{22} \cdots 1_{rr}|$, that is, for $(H_1:H_2)$ is 2^r.

As examples, consider the cases $n=5$ and 7. The case $n=5$ has been worked out by O. Taussky [8] by a different method.

(1) $n=5$. Let ζ be a primitive 5th root of unity. From Theorem 5, $b(5)=1=r$. Fueter [1, p. 186] showed that $\epsilon(\zeta)=\zeta^2+\zeta^3$ is a fundamental unit of E of infinite order, hence $(\epsilon(\zeta), \epsilon(1))=f_1$ can be chosen as a basis of F. From Theorem 4, $(F:F_1')=4$ so that $f_1^{(1)}=f_1^4=(\epsilon(\zeta)^4, \epsilon(1)^4)$, where $\epsilon(\zeta)^4=6+4\zeta+\zeta^2+\zeta^3+4\zeta^4$ $=3+\zeta-2\zeta^2-2\zeta^3+\zeta^4$. (Note that, since $\epsilon(1)=2$, the smallest exponent k such that $2^k \equiv 1 \pmod 5$, is $k=4$.) The group of nonzero residues modulo p is cyclic so that $f_1^{(1)}$ can be taken as a basis of F_1' and the circulant $C=[3, 1, -2, -2, 1]$ is a basis of H_1. But C is positive definite so that for the case $n=5$, $H_1=H_2$. Furthermore, $C=[1, 0, -1, -1, 0]^2$ which implies that there is only one class of symmetric positive definite unimodular 5×5 circulants with respect to congruence over rational integral circulants.

(2) $n=7$. Let ζ be a primitive 7th root of unity. From Theorem 5, $b(7)=2=r$. Fueter [1, p. 186] showed that $\epsilon(\zeta)=1+\zeta+\zeta^6$ and $\delta(\zeta)=1+\zeta^3+\zeta^4$ are fundamental units of E of infinite order, hence $(\epsilon(\zeta), \epsilon(1))=f_1$ and $(\delta(\zeta), \delta(1))=f_2$ can be chosen as a basis of F. From Theorem 4, $(F:F_1')=6$ so that

$$f_1^{(1)}=f_1^{k_{11}} \cdot f_2^{k_{12}}$$

and

$$f_2^{(1)}= \qquad f_2^{k_{22}},$$

where $|k_{11} \cdot k_{22}|=6$ form a basis of F_1'. Since $\delta(1)=3$ it follows that k_{22} must satisfy $3^{k_{22}} \equiv 1 \pmod 7$, hence $k_{22}=6$ and $f_2^{(1)}=f_2^6$ is a basis element of F_1'. Also, $k_{11}=\pm1$. Let $k_{11}=1$. Since $\epsilon(1)=3$ it follows that k_{12} must satisfy $3 \cdot 3^{k_{12}} \equiv 1 \pmod 7$, hence $k_{12}=5$ and $f_1^{(1)}=f \cdot f_2^5$ is a second basis element of F_1'. Now

$$f_1^{(1)}=113+102\zeta+96\zeta^2+110\zeta^3+110\zeta^4+96\zeta^5+102\zeta^6$$

$$=9-2\zeta-8\zeta^2+6\zeta^3+6\zeta^4-8\zeta^5-2\zeta^6,$$

since $\epsilon(1) \cdot \delta(1)^5=3^6=1+104 \cdot 7$, and

$$f_2^{(1)}=141+96\zeta+71\zeta^2+127\zeta^3+127\zeta^4+71\zeta^5+96\zeta^6$$

$$=37-8\zeta-33\zeta^2+23\zeta^3+23\zeta^4-33\zeta^5-8\zeta^6,$$

since $\delta(1)^6=3^6=1+104.7$.

Thus the circulants

$$C_1=[9, -2, -8, 6, 6, -8, -2]$$

$$C_2=[37, -8, -33, 23, 23, -33, -8]$$

can be taken as a basis of H_1.

In a similar manner it can be shown that

$$f_1^{(2)}=f_1^{(1)2} \text{ and } f_2^{(2)}=f_2^{(1)}$$

form a basis of F_2 so that

$$D_1=C_1^2=[289, -64, -260, 180, 180, -260, -64]$$

$$D_2=C_2=[37, -8, -33, 23, 23, -33, -8]$$

form a basis of H_2. A more convenient choice of basis would be

$$D_1'=C_1^2 \cdot C_2^{-1}=[3, 0, -2, 1, 1, -2, 0]$$

$$D_2'= \qquad C_2=[37, -8, -33, 23, 23, -33, -8].$$

In the latter case,

$$D_1'=[-1, 0, 1, 0, 0, 1, 0]^2$$

$$D_2'=[-3, 1, 3, -2, -2, 3, 1]^2$$

so that there is only one class of symmetric positive definite unimodular 7×7 circulants with respect to congruence over rational integral circulants.

Number of Classes of Circulants. M. Kneser [3, p. 250] lists the class number of positive definite quadratic forms in n variables for $1 \leq n \leq 16$ and with determinant 1. The number of classes of circulants in H_2 is less than or equal to this class number for each n. In particular, it is shown that there is only one class H_2 for $n \leq 7$. M. Newman and O. Taussky [7] showed there are two classes for $n=8$. In private communications M. Kneser proved there is one class for $n=9$; M. Newman proved there are two classes for $n=12$; and E. C. Dade and O. Taussky found one class for all prime $p<100$ except $p=29$. The number of classes for other values of n is not known but an upper bound can be obtained.

THEOREM 8. $(H_1:H_2) \leq 2^r$, *where* r *is the number of basis elements of* H_1.

PROOF: Let H_0 be the set of all elements C of H_1 such that $C \equiv I$; that is $C=A'A$ where A is an $n\times n$ unimodular rational integral circulant. Then

(i) If $C \epsilon H_1$, then $C^2 \epsilon H_0$ (since $C^2=C'IC$).

(ii) H_0 is a subgroup of H_1.

(iii) $(H_1:H_0)$ is the number of classes of circulants of H_1, where congruence is over the unimodular rational integral circulants.

By Theorem 5, the number of basis elements of H_1 is $r=\left[\frac{n}{2}\right]+1-\sigma_0(n)$. If $C_1, \ldots, C_r$ are basis elements

of H_1, then because of (i) and (ii) any element C of H_1 can be written in the form

$$C = C_1^{\theta_1} \cdot C_2^{\theta_2} \cdot \cdots \cdot C_r^{\theta_r} \cdot C_0$$

where $C_0 \epsilon H_0$ and $\theta_i = 0$ or 1 for $1 \leq i \leq r$. This implies that the order of H_1/H_0 is 2^s where $s \leq r$, hence 2^r is an upper bound for the class number in (iii). But the number of circulants of H_1 with respect to integral congruence is not greater than the number of classes with respect to congruence over circulants, so that 2^r is actually an upper bound for this class number. Thus $(H_1 : H_0) \leq 2^r$ and since H_0 is a subgroup of H_2 it follows that $(H_1 : H_2) \leq 2^r$.

Appendix

The following list includes the notation and definitions of all sets referred to in the paper.

Set Definition

G = All rational integral unimodular $n \times n$ circulants.

G_1 = Symmetric elements of G.

G_2 = Positive definite elements of G_1.

E = All units in $R(\zeta)$.

E_1 = Real elements of E.

E_2 = Totally positive elements of E_1.

E_1' = Largest aperiodic subgroup of E_1.

$E_1'' = \{\epsilon(\zeta) \epsilon E_1' | \epsilon(1) \equiv 1 \pmod{p}\}$.

H = Largest aperiodic subgroup of G.

H_1 = Elements of H all of whose eigenvalues are elements of E_1'.

$H_2 = H_1 \cap G_2$.

$\mathcal{F} = \theta(G) = \{(\epsilon(\zeta^{d_1}), \ldots, \epsilon(\zeta^{d_m})) | d_1, \ldots, d_m$ are positive divisors of n; $\epsilon(\zeta) \epsilon E\}$.

$F = \theta(H)$.

$F_1' = \theta(H_1)$, when $n \neq p^\alpha$, $= \{(\epsilon(\zeta^{d_1}), \ldots, \epsilon(\zeta^{d_m})) | \epsilon(\zeta^{d_i}) \epsilon E_1', 1 \leq i \leq m\}$.

$F' = \theta(H_1)$, when $n = p^\alpha$, $= \{(\epsilon(\zeta^{d_1}), \ldots, \epsilon(\zeta^{d_m})) | \epsilon(\zeta^{d_i}) \epsilon E_1'', 1 \leq i \leq m\}$.

$F_2 = \theta(H_2)$.

References

[1] R. Fueter, Synthetische Zahlentheorie, Berlin (1921).
[2] E. Hecke, Vorlesungen uber die Theorie der algebraischen Zahlen, Chelsea, New York (1948).
[3] M. Kneser, Klassenzahlen definiter quadratischer formen, Arch. Math. **VIII**, 241–250 (1957).
[4] W. LeVeque, Topics in Number Theory, Vol. **I** (Addison-Wesley, Reading, Mass., 1956).
[5] T. Nagell, Introduction to Number Theory, (John Wiley & Sons, New York, N.Y., 1951).
[6] M. Newman, Circulant quadratic forms, Proc. Boulder Conference, 1959.
[7] M. Newman and O. Taussky, Classes of positive definite unimodular circulants, Canad. J. Math. **9**, 71–73 (1957).
[8] O. Taussky, Unimodular integral circulants, Math. Z. **63**, 286–289 (1955).
[9] H. Zassenhaus, The Theory of Groups (Chelsea, New York, 1949).

(Paper 69B4–160)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 69B, No. 4, October–December 1965

A Generalization of a Result of Newman on Multipliers of Difference Sets

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(June 17, 1965)

A theorem of M. Newman states that if v, k, λ, are the parameters for a difference set D, and $k-\lambda=p$ or $2p$ (p a prime) then p is a multiplier of D. This theorem is generalized to the case of an abelian difference set and several consequences are noted.

Key Words: Abelian, multipliers, block designs, difference sets.

1. Introduction

A *difference set* with parameters (v, k, λ, n) is a subset

$$D=\{d_1, \ldots, d_k\}$$

of k distinct elements of a (multiplicative) group G with finite order v, such that every nonidentity element g in G can be expressed in exactly λ ways as

$$d_i^{-1}d_j=g, \qquad 1 \leqq i, j \leqq k.$$

The parameter n is defined by

$$n=k-\lambda.$$

Counting the total number of nonidentity "differences," $d_i^{-1}d_j$, in two ways yields

$$k(k-1)=\lambda(v-1). \tag{1}$$

The difference set D is said to be *abelian* (*cyclic*) in case the group G is abelian (cyclic). The *exponent*, v^*, of the difference set D is the least common multiple of the orders of the elements of G. An integer t is a *multiplier* of the difference set

$$D=\{d_1, \ldots, d_k\}$$

in case the sets

$$D(t)=\{d_1^t, \ldots, d_k^t\}$$

$$gD=\{gd_1, \ldots, gd_k\}$$

are identical, apart from order, for some group element g in G.

Newman [5][2] has proved the following result.

THEOREM 1. *Let* D *be a cyclic difference set with parameters* (v, k, λ, n). *Suppose*

$$n=2p, \quad (7p, v)=1$$

where p *is a prime. Then* p *is a multiplier of* D.

Theorem 1 can be generalized in two ways. First of all, it can be generalized to abelian difference sets. Secondly, as H. B. Mann has pointed out, theorem 1 can be combined with the following multiplier theorem.

THEOREM 2. *Let* D *be an abelian difference set with parameters* (v, k, λ, n) *and exponent* v^*. *Suppose*

$$n_1 \mid n, \quad (n_1, v)=1, \quad n_1>\lambda, \quad n_1=p_1^{e_1}\cdots p_s^{e_s}$$

where the p_i *are distinct primes. If there exist integers* $f_1, \ldots, f_s$ *such that*

$$t \equiv p_1^{f_1} \equiv \cdots \equiv p_s^{f_s} \pmod{v^*}$$

then t *is a multiplier of* D.

Theorem 2 was proven for cyclic difference sets by Hall [2]. It was generalized to abelian difference sets by Menon [4]. More recently, Mann [3] has given another proof of theorem 2.

These two generalizations of theorem 1 yield:

THEOREM 3. *Let* D *be an abelian difference set with parameters* (v, k, λ, n) *and exponent* v^*. *Suppose*

$$n=2n_1, \quad (7n_1, v)=1, \quad n_1=p_1^{e_1}\cdots p_s^{e_s}$$

where the p_i *are distinct primes. If there exist integers* $f_1, \ldots, f_s$ *such that*

$$t \equiv p_1^{f_1} \equiv \cdots \equiv p_s^{f_s} \pmod{v^*}$$

then t *is a multiplier of* D.

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[2] Figures in brackets indicate the literature references at the end of this paper.

A special case of theorem 3 is worthy of note.

COROLLARY. *Let* D *be an abelian difference set with parameters* (v, k, λ, n). *If*

$$n = 2p^e, \qquad e \geqq 1, \qquad (7p, v) = 1$$

where p *is a prime, then* p *is a multiplier of* D.

This paper is devoted to the proof of theorem 3.

2. Preparatory Lemmas

Let R_G denote the group ring of the finite multiplicative abelian group G over the rational integers. The elements of R_G are of the form

$$\sum_{g \in G} a_g g$$

where the coefficients a_g are integral. Addition in R_g is component addition of the coefficients

$$\sum_g a_g g + \sum_g b_g g = \sum_g (a_g + b_g) g.$$

Multiplication in R_G is the usual multiplication in an associative algebra with basis consisting of the elements of G

$$\left(\sum_g a_g g\right)\left(\sum_{\bar{g}} b_{\bar{g}} \bar{g}\right) = \sum_h h \sum_{g\bar{g}=h} a_g b_{\bar{g}}.$$

No confusion will result if we let G denote the element

$$G = \sum_g g$$

in R_G that has every coefficient equal to one. Similarly, if the difference set D in G consists of the k elements $d_1, \ldots, d_k$ we shall write D to denote the element

$$D = d_1 + \cdots + d_k$$

in R_G. For any integer t and any group element g we define

$$D(t) = d_1^t + \cdots + d_k^t$$

$$tD = td_1 + \cdots + td_k$$

$$gD = gd_1 + \cdots + gd_k.$$

The definition of a difference set implies that

$$D(-1)D = n + \lambda G \tag{2}$$

where we have surpressed the identity element of G on n. Also

$$DG = kG. \tag{3}$$

The integer t is a multiplier of the difference set D if and only if

$$D(t) = gD \tag{4}$$

for some g in G.

LEMMA 1. *Let* D *and* D* *be difference sets with parameters* (v, k, λ, n) *in the same group* G. *Let*

$$F = D(-1)D^* - \lambda G.$$

Then

(i) $FG = nG$

(ii) $F(-1)F = n^2$

(iii) $FD = nD^*$.

If F *has nonnegative coefficients, then*

$$gD = D^*$$

for some g *in* G.

PROOF. Parts (i), (ii), and (iii) can be verified by straightforward computations using eqs (1), (2), and (3). If F has nonnegative coefficients, then part (ii) implies that F has exactly one nonzero coefficient, say

$$F = ng, \qquad g \in G.$$

Then part (iii) implies that

$$gD = D^*$$

as desired.

LEMMA 2. *Let* G *be a finite abelian group with order* v *prime to* 2 *and* 7. *Let* E *be an element in the group ring* R_G *such that*

(i) $EG = 2G$

(ii) $E(-1)E = 4$.

Then E *has nonnegative coefficients.*

PROOF. Let

$$E = \sum_{g \in G} a_g g$$

with a_g integral. Hypothesis (i) implies

$$\sum_g a_g = 2 \tag{5}$$

while hypothesis (ii) implies

$$\sum_g a_g^2 = 4 \tag{6}$$

and

$$\sum_{g^{-1}\bar{g}=h} a_g a_{\bar{g}} = 0, \qquad h \neq 1. \tag{7}$$

Assume that E has a negative coefficient. Then eqs (5) and (6) imply that E has one coefficient equal to minus one, three coefficients equal to plus one, and the remaining coefficients zero. Thus

$$E = -w + x + y + z \tag{8}$$

for distinct group elements w, x, y, z in G. Letting $h = w^{-1}x, w^{-1}y, w^{-1}z$ in eq (7) we obtain either two or four nonzero terms in the left-hand sum. Suppose four nonzero terms occur for $h = w^{-1}x$. Then there are exactly three possibilities, namely

$$h = w^{-1}x = x^{-1}w = y^{-1}z = z^{-1}y$$
$$h = w^{-1}x = x^{-1}y = y^{-1}z = z^{-1}w$$
$$h = w^{-1}x = x^{-1}z = y^{-1}w = z^{-1}y.$$

In each of these three possibilities, $h^4 = 1$. Thus $h = 1$, since v is odd; a contradiction. Therefore, by symmetry among x, y, z, we conclude that exactly two nonzero terms occur in eq (7) for $h = w^{-1}x, w^{-1}y, w^{-1}z$. Now eq (7) implies that there are four possible values for each of $w^{-1}x, w^{-1}y, w^{-1}z$.

$$w^{-1}x = x^{-1}y, x^{-1}z, y^{-1}z, z^{-1}y$$
$$w^{-1}y = x^{-1}z, y^{-1}x, y^{-1}z, z^{-1}x$$
$$w^{-1}z = x^{-1}y, y^{-1}x, z^{-1}x, z^{-1}y$$

We shall use the symbol "↔" to indicate that a contradiction has been obtained.

Case I: $w^{-1}x = x^{-1}y$.

Case I_A: $w^{-1}x = x^{-1}y$, $w^{-1}z = x^{-1}y$.
Then $x^2 = wy = xz \Rightarrow x = z$ ↔.

Case I_B: $w^{-1}x = x^{-1}y$, $w^{-1}z = y^{-1}x$.
Then $w^{-1}x = x^{-1}y = z^{-1}w$ so eq (7) contains more than two nonzero terms ↔. .

Case I_C: $w^{-1}x = x^{-1}y$, $w^{-1}z = z^{-1}y$.
Then $x^2 = wy = z^2 \Rightarrow x = z$ ↔.

Case I_D: $w^{-1}x = x^{-1}y$, $w^{-1}z = z^{-1}x$.
Applying the permutation $x \to z$, $y \to x$, $z \to y$ to Cases I_A, I_B, I_C we see that $w^{-1}z = z^{-1}x$ implies $w^{-1}y \neq z^{-1}x$, $x^{-1}z$, $y^{-1}x$. Therefore $w^{-1}x = x^{-1}y$ implies that $w^{-1}z = z^{-1}x$ and $w^{-1}y = y^{-1}z$. Eliminating w^{-1} among these three equations yields $x^{-2}y = y^{-2}z = z^{-2}x$. Now eliminating an appropriate power of x yields $y^7 = z^7$. Thus $y = z$, since $(v, 7) = 1$; a contradiction.
Therefore Case I is impossible. By the symmetry among x, y, z we have

$$w^{-1}x \neq x^{-1}y, x^{-1}z$$
$$w^{-1}y \neq y^{-1}z, y^{-1}x$$
$$w^{-1}z \neq z^{-1}x, z^{-1}y.$$

Thus there are eight possibilities remaining, namely

$$w^{-1}x = y^{-1}z, z^{-1}y$$
$$w^{-1}y = x^{-1}z, z^{-1}x$$
$$w^{-1}z = x^{-1}y, y^{-1}x.$$

By the symmetry between y and z we can assume

$$w^{-1}x = y^{-1}z.$$

Either $w^{-1}z = x^{-1}y$, or else $w^{-1}z = y^{-1}x$. In the first case

$$w^{-1}x = y^{-1}z = wx^{-1} \Rightarrow w^2 = x^2 \Rightarrow w = x \leftrightarrow,$$

while in the second case

$$w^{-1}y = x^{-1}z = wy^{-1} \Rightarrow w^2 = y^2 \rightarrow w = y \leftrightarrow.$$

We have now exhausted all possibilities. Therefore E cannot have a negative coefficient, and the proof is complete.

LEMMA 3. *Let* D *be an abelian difference set with parameters* (v, k, λ, n) *in the group* G. *Let* p *be a prime such that*

$$p^e | n, \qquad (p, v) = 1.$$

Then for every integer f, *the coefficients of*

$$F = D(-1)D(p^f) - \lambda G$$

are divisible by p^e.

PROOF. Lemma 3 appears as a part of the proof of corollary 4.1 of Mann [3]. Alternatively, lemma 3 is a special case of eq (3.9) of Menon [4].

3. Theorem

THEOREM 3. *Let* D *be an abelian difference set with parameters* (v, k, λ, n) *and exponent* v^*. *Suppose*

$$n = 2n_1, \qquad (7n_1, v) = 1, \qquad n_1 = p_1^{e_1} \cdots p_s^{e_s}$$

where the p_i *are distinct primes. If there exist integers* $f_1, \ldots, f_s$ *such that*

$$t \equiv p_1^{f_1} \equiv \cdots \equiv p_s^{f_s} \pmod{v^*}$$

then t *is a multiplier of* D.

PROOF. If D is a difference set in the group G, then $G - D$ is also a difference set. Clearly any multiplier of D is also a multiplier of $G - D$. Furthermore, one of these difference sets has $\lambda > n$. Consequently, if n_1 is even, then theorem 3 is a special case of theorem 2. Now assume n_1 is odd. Then $n = 2n_1$ is not a square. In this case it is well known (e.g. theorem 3 of Chowla and Ryser [1]) that v is odd.

Let

$$F = D(-1)D(t) - \lambda G.$$

Since

$$D(p_i^t) = D(t), \qquad (i = 1, \ldots, s),$$

lemma 3 implies that the coefficients of F are divisible by n_1. Let

$$E = n_1^{-1}F.$$

Parts (i) and (ii) of lemma 1 imply that E satisfies the hypotheses (i) and (ii) of lemma 2. Therefore E, and consequently F, has nonnegative coefficients. Then by lemma 1,

$$gD = D(t)$$

for some group element g. Thus t is a multiplier of D.

4. References

[1] S. Chowla and H. J. Ryser, Combinatorial problems, Can. J. Math. **2**, 93–99 (1950).

[2] Marshall Hall, Jr., A survey of difference sets, Proc. Amer. Math. Soc. **7**, 975–986 (1956).

[3] H. B. Mann, Balanced incomplete block designs and abelian difference sets, Ill. J. Math. **8**, 252–261 (1964).

[4] P. Kesava Menon, Difference sets in abelian groups, Proc. Amer. Math. Soc. **11**, 368–376 (1960).

[5] Morris Newman, Multipliers of difference sets, Can. J. Math. **15**, 121–124 (1963).

(Paper 69B4–161)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 69B, No. 4, October–December 1965

The Bridge Tournament Problem and Calibration Designs for Comparing Pairs of Objects

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(August 17, 1965)

The classical tournament problem calls for arranging v individuals into teams of p players so that a player is teamed the same number of times with each of the other players and also that each player is pitted equally often against each of the other players. The play of the tournament results in the determination of difference in performance of the various pairings of the groups. In the special case when $p=2$ each team consists of two players and the designs are called bridge tournament designs.

In high precision calibration one can measure only the difference between two nominally equal groups so that if v objects are to be intercompared in groups of p objects, then the solutions to the tournament problem provide schedules for the grouping. These designs are useful in weighing and any other measurements where the objects to be measured can be combined into groups without loss of precision or accuracy in the comparisons.

This paper presents general methods for constructing of bridge tournament designs, i.e., for the case when $p=2$, for all $v \leq 50$.

Key Words: Calibration, calibration designs, combinatorial analysis, difference sets, experiment designs, incomplete block designs, tournaments, weighing designs.

1. Introduction

The classical tournament problem calls for arranging v individuals into teams of p players, so that each player is teamed the same number of times with each of the other players, and also each player is pitted equally often against each of the other players. Consistent with these conditions one would like to minimize the number of matches. Such an arrangement may be called a tournament design. Each match corresponds to a block of this design, the block being divided into two half-blocks corresponding to the two teams. When the tournament is played according to this design, it facilitates the determination of the difference in performance between the various pairs of players.

In high precision calibration one can measure the difference between two nominally equal groups so that if v objects are intercompared in groups of p objects then tournament designs provide schedules for grouping into sets. These designs are useful in weighing and other measurements where the objects to be measured can be combined into groups without loss of precision or accuracy in the comparisons.

In the special case when $p=2$, each team consists of two players, which is the situation in a bridge match. The corresponding designs can then be called bridge tournament designs. When used for calibration, two pair of objects are compared with each other.

In this paper we give general methods for constructing bridge tournament designs, and obtain in particular all designs for $v \leqq 50$. The statistical analysis for the corresponding calibration designs will appear elsewhere. The tournament designs for $p>2$ will be considered in a separate communication. For previous work on the same problem, reference should be made to [7,[1] 10, 13, and 14].

2. Parameters for Tournament Designs

Let there be v players or objects. We have to arrange them in b blocks of size $2p$, each block consisting of two half-blocks of size p. Two objects appear in the same half block λ_1 times, and in opposite half-blocks of the same block λ_2 times. Then

$$v,\ b,\ r,\ p,\ \lambda_1,\ \lambda_2, \tag{2.1}$$

are said to be the parameters of the tournament design, where r is the number of blocks in which each object appears.

Consider the r blocks in which a given object θ appears. Then there are $r(p-1)$ other objects in the half-blocks containing θ. Since each of the $v-1$ objects other than θ, appears λ_1 times in the same half-block as θ,

$$\lambda_1(v-1)=r(p-1). \tag{2.2}$$

Similarly

$$\lambda_2(v-1)=rp. \tag{2.3}$$

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[1] Figures in brackets indicate the literature references at the end of this paper.

Hence $r=(\lambda_2-\lambda_1)(v-1)$, which shows that r must be divisible by $v-1$. We can take $r=\beta(v-1)$. Let there be b blocks (or matches). Then counting the number of objects in the b blocks in two different ways we have

$$2pb=vr=v(v-1)\beta.$$

Hence

$$b=\beta v(v-1)/2p.$$

Let h be the highest common factor of $v(v-1)$ and $2p$ and let $2p=hn$. Then $\beta=\lambda_2-\lambda_1$ must be divisible by n, hence the least possible value of β is n. If the corresponding design exists we shall call it minimal in the sense that no smaller number of blocks could possibly lead to a balanced design, i.e., integer values for λ_1 and λ_2.

The parameters of a minimal design are

$$v,\ b=v(v-1)/h,\ r=n(v-1),\ p,$$

$$\lambda_1=n(p-1),\ \lambda_2=np, \qquad (2.4)$$

where h is the highest common factor of $v(v-1)$ and $2p=hn$.

Now consider the special case $p=2$. In this case $h=4$, $n=1$, if $v=4t+1$ or $4t$, and $h=2$, $n=2$ if $v=4t+3$ or $4t+2$. Hence we have the following four series of minimal bridge tournament designs.

(A) $v=4t+3,\ b=(4t+3)(2t+1),$

$$r=2(4t+2),\ p=2,\ \lambda_1=2,\ \lambda_2=4,$$

(B) $v=4t+1,\ b=t(4t+1),\ r=4t,$

$$p=2,\ \lambda_1=1,\ \lambda_2=2,$$

(C) $v=4t+2,\ b=(2t+1)(4t+1),$

$$r=2(4t+1),\ p=2,\ \lambda_1=2,\ \lambda_2=4,$$

(D) $v=4t,\ b=t(4t-1),\ r=4t-1,$

$$p=2,\ \lambda_1=1,\ \lambda_2=2. \qquad (2.5)$$

We shall show that an infinity of designs exist for each series. In particular all the designs for $v\leqq 50$ exist, and will be explicitly obtained.

3. The Method of Symmetrically Repeated Differences

Tournament designs are very closely related with balanced incomplete block (BIB) designs.

A BIB design is an arrangement of v^* objects in b^* blocks or sets such that (i) each block contains exactly k^* different objects (ii) each object appears in exactly r^* blocks (iii) any pair of distinct objects appear together in exactly λ^* blocks. The BIB design is then said to have parameters $v^*, b^*, r^*, k^*, \lambda^*$. It is evident that the necessary and sufficient condition for the existence of a tournament design with parameters (2.1) is the existence of a BIB design with parameters

$$v^*=v,\ b^*=b,\ r^*=r,\ k^*=2p,\ \lambda^*=\lambda_1+\lambda_2, \qquad (3.1)$$

each of whose blocks can be divided into two half-blocks such that the half-blocks form a BIB design with parameters

$$v_0=v,\ b_0=2b,\ r_0=r,\ k_0=p,\ \lambda_0=\lambda_1. \qquad (3.2)$$

The method of symmetrically repeated differences which was originally developed by Bose [1], in connection with the construction of BIB designs, can be adapted to the construction of tournament designs. An excellent exposition of the method will be found in Mann [11]. We shall give here the necessary definitions and quote the two basic theorems, without introducing the concepts of mixed differences which will not be explicitly needed in this paper.

Consider a module M with n elements. If a_1 and a_2 are any elements of M we say that the elements $\pm(a_1-a_2)$ are the differences arising from the pair a_1, a_2. Let the objects be put in one-to-one correspondence with the elements of M. Given a block B with m elements $a_1, a_2, \ldots, a_m$, the $m(m-1)$ differences $\pm(a_i-a_j)$, $i, j=1, 2, \ldots, m$, $i\neq j$, arising from all distinct pairs of objects in the block, are called the differences arising from the block. Given a set of blocks such that among the differences arising from the blocks of the set, each nonzero element of M occurs exactly λ times, we say that the differences arising from the set of blocks are symmetrically repeated λ times. From the block $B=(a_1, a_2, \ldots, a_m)$ we can form a set of n blocks $(a_1+\theta, a_2+\theta, \ldots, a_m+\theta)$, where θ runs over all the different elements of M. This set of n blocks is said to be obtained by developing the initial block B. We can now enunciate the following theorem:

THEOREM 1. *Let* M *be a module containing* v* *elements, which have been put in one-to-one correspondence with a set of* v* *objects. If there exists a set of* t *blocks*

$$B_1, B_2, \ldots, B_t, \qquad (3.3)$$

such that (i) Each block contains k* *distinct objects (ii) the differences arising from the blocks are symmetrically repeated* λ* *times, then we get a BIB design with parameters*

$$v^*,\ b^*=v^*t,\ r^*=k^*t,\ k^*,\ \lambda^* \qquad (3.4)$$

by developing the initial blocks (3.3).

THEOREM 2. *Let* M *be a module containing* n *elements, which have been put in one-to-one correspondence with a set of* n *objects. To these adjoin a new object* ∝. *If it is possible to find a set of* g+s *blocks*

$$B_1, B_2, \ldots, B_g, B_1', B_2', \ldots, B_s'; \qquad (3.5)$$

such that (i) Each of the blocks $B_1, B_2, \ldots, B_g$ *contains*

k^* *distinct objects which are all different from* ∞ *while each of the blocks* $B_1', B_2', \ldots B_s'$ *contains* ∞ *and* k^*-1 *other distinct objects, (ii) The differences arising from the blocks* $B_1, B_2, \ldots B_t, B_1'', B_2'', \ldots, B_s''$, *where the blocks* B_j'' *are obtained from* B_j' $(j=1, 2, \ldots s)$ *by cutting out the adjoined object* ∞, *are symmetrically repeated* λ^* *times, (iii)* $k^*g+\lambda^*=ns$, $\lambda^*=(k^*-1)s$ *then we get a BIB design with parameters*

$$v^*=n+1,\ b^*=n(g+s),\ r^*=ns,\ k^*=k,\ \lambda^*=\lambda,$$

by developing the blocks (3.5), where ∞ *remains unchanged during development.*

For a proof of slightly more general theorems see Bose [1], pp. 366–372 and Mann [11], pp. 115–118.

4. Designs Belonging to the Series (A), When $4t+3$ is a Prime Power

In the remainder of this paper we shall consider only bridge tournament designs, i.e., the special case $p=2$ of general tournament designs. When the module M is a commutative ring or a field it will be be convenient to use the notation

$$\{(a_1, a_2), (b_1, b_2)\} \oplus (c_1, c_2, \ldots c_u). \tag{4.1}$$

to denote the set of blocks

$$\{(a_1c_i, a_2c_i), (b_1c_i, b_2c_i)\},\ i=1, 2, \ldots, u. \tag{4.2}$$

If $4t+3=q$ is a prime power, we can identify the v objects or players with elements of the Galois field $GF(q)$. Let x be a primitive element of $GF(q)$, and let a_1, a_2, b_1, b_2 be any four nonzero distinct elements of $GF(q)$.

Now $x^{4t+2}=1$ and $x^{2t+1}=-1$, so that -1 is an odd power of x. It follows that if c and d are any distinct elements of $GF(q)$ the differences arising from the pairs

$$(c, d), (cx^2, dx^2), \ldots (cx^{4t}, dx^{4t}),$$

are symmetrically repeated once.

Now consider the set of $2t+1$ blocks

$$\{(a_1, a_2), (b_1, b_2)\} \oplus (1, x^2, x^4, \ldots x^{4t}). \tag{4.3}$$

If we take the $4t+2$ half-blocks from (4.3) as initial blocks, the differences arising from these are symmetrically repeated twice. Hence we get a BIB design with parameters

$$v_0=4t+3,\ b_0=2(4t+3)(2t+1),$$
$$r_0=4(2t+1),\ k_0=2,\ \lambda_0=2.$$

Similarly if we take the $2t+1$ blocks in (4.3) as initial blocks (without partitioning into half-blocks), we get a BIB design with parameters

$$v^*=4t+3,\ b^*=(4t+3)(2t+1),$$
$$r^*=4(2t+1),\ k^*=4,\ \lambda^*=6.$$

It follows that if we develop the initial blocks (4.3), keeping the half-blocks intact, we get a bridge tournament design belonging to the series A.

In particular we get the solutions for $v=7, 11, 19, 23, 27, 31, 43, 47$. For $v \leq 50$ this leaves only the values 15, 35, and 39 of the form $4t+3$. These will be considered in section 14.

EXAMPLE (1). Let $t=1$. The required design has the parameters $v=7$, $b=21$, $r=12$, $p=2$, $\lambda_1=2$, $\lambda_2=4$. Now 3 is a primitive element of $GS(7)$. Hence the design can be developed from the initial blocks

$$\{(1, 2), (3, 4)\} \oplus (1, 2, 4)$$

which leads to the design

1 2 3 4	2 4 6 1	4 1 5 2
2 3 4 5	3 5 0 2	5 2 6 3
3 4 5 6	4 6 1 3	6 3 0 4
4 5 6 0	5 0 2 4	0 4 1 5
5 6 0 1	6 1 3 5	1 5 2 6
6 0 1 2	0 2 4 6	2 6 3 0
0 1 2 3	1 3 5 0	3 0 4 1

EXAMPLE (2). Let $t=2$. The required design has parameters $v=11$, $b=55$, $r=20$, $p=2$, $\lambda_1=2$, $\lambda_2=4$. A primitive element of $GF(11)$ is 2. The design can be developed from the initial blocks

$$\{(1, 2), (3, 4)\} \oplus (1, 4, 5, 9, 3).$$

5. Designs Belonging to the Series (B), When $4t+1$ is a Prime Power

Let $4t+1=q$ be a prime power. Now Mann [11], pp. 118–119, has shown that if x is a primitive element of $GS(q)$, where $q=4t+1$, then there exist odd integers α and β such that

$$\frac{x^\alpha+1}{x^\alpha-1}=x^\beta. \tag{5.1}$$

Consider the set of t blocks

$$\{(1, x^{2t}), (x^\alpha, x^{\alpha+2t})\} \oplus (1, x^2, x^4, \ldots, x^{2t-2}). \tag{5.2}$$

Now $x^{4t}=1$, $x^{2t}=-1$. Let $x^{2t}-1=x^s$. Then the differences arising from the $2t$ half-blocks in (5.2) are

$$x^{s+2i}, x^{s+2i+\alpha},\ i=0, 2, \ldots 2t-2. \tag{5.3}$$

Since α is odd the differences are symmetrically repeated once. Hence the $2t$ half-blocks in (5.2) on development give the BIB design.

$$v_0=4t+1,\ b_0=2t(4t+1),\ r_0=4t,\ k_0=2,\ \lambda_0=1. \tag{5.4}$$

Again consider the differences arising from the t blocks (5.2), disregarding the partitions into half-blocks. Then in addition to (5.3), we will have the differences arising from cross pairs, i.e., pairs whose members belong to different half-blocks. Let $x^a - 1 = x^c$, $x^a + 1 = x^d$. Then these differences can be written as

$$x^{c+2i},\ x^{c+2t+2i},\ x^{d+2i},\ x^{d+2t+2i},\ i = 0, 1, \ldots, 2t-2. \tag{5.5}$$

If we remember that in virtue of (5.1), $c-d$ is odd we see that in (5.5) each nonzero element of $GF(q)$ occurs twice. Hence the differences from the blocks (5.2) are symmetrically repeated thrice. On developing these blocks we get a BIB design with parameters,

$$v^* = 4t+1,\ b^* = t(4t+1),\ r^* = 4t,\ k^* = 4,\ \lambda^* = 3. \tag{5.6}$$

Hence if we develop the initial blocks (5.2), keeping the half-blocks intact we get a bridge tournament design belonging to the series (B).

In particular we get solutions for $v = 5, 9, 13, 17, 25, 29, 37, 41, 49$. If $v \leqslant 50$, this leaves only the values 21, 33 and 45 of the form $4t+1$. These will be considered in section 11.

EXAMPLE (1). Let $t = 1$. Then the required design has parameters $v = 5$, $b = 5$, $r = 4$, $p = 2$, $\lambda_1 = 1$, $\lambda_2 = 2$. A primitive element of $GF(5)$ is 2, and

$$\frac{2+1}{2-1} = 3 = 2^3.$$

Hence $\alpha = 1$, $\beta = 3$, and the initial block is

$$\{(1, 4), (2, 3)\}.$$

The complete design obtained by developing it has the blocks

$$\{(1, 4), (2, 3)\},\ \{(2, 5), (3, 4)\},\ \{(3, 1), (4, 5)\},\ \{(4, 2), (5, 1)\},\ \{(5, 3), (1, 2)\}. \tag{5.7}$$

EXAMPLE (2). Let $t = 2$. Then the required design has parameters $v = 9$, $b = 18$, $r = 8$, $p = 2$, $\lambda_1 = 1$, $\lambda_2 = 2$. Let x be a primitive element of $GF(3^2)$ with minimum equation $x^2 + x + 2 = 0$. Then

$$\frac{x+1}{x-1} = x,$$

whence $\alpha = 1$, $\beta = 1$. The design is obtained by developing the initial blocks

$$\{(1, x^4), (x, x^5)\},\ \{(x^2, x^5), (x^3, x^7)\}.$$

EXAMPLE (3). When $t = 3$, the required design has the parameters $v = 13$, $b = 39$, $r = 12$, $p = 2$, $\lambda_1 = 1$, $\lambda_2 = 2$. Now 2 is a primitive element of $GF(13)$ and

$$\frac{2^3+1}{2^3-1} = 2^9.$$

Hence we can take $\alpha = 3$, $\beta = 9$. The design is obtained by developing the initial blocks

$$\{(1, 12), (8, 5)\},\ \{(4, 9), (6, 7)\},\ \{(3, 10), (11, 2)\}.$$

6. Designs Belonging to the Series (C), When $4t+1$ is a Prime Power

Let $4t+1 = q$ where q is a prime power. We identify each element of $GF(q)$ with one object and take an additional object ∞. To construct the initial blocks for the required design, we shall use the solution for series (B) already obtained in section 5. Let α and β be as in section 5. Let the initial block $\{(1, x^{2t}), (x^a, x^{a+2t})\}$ be replaced by two blocks

$$\{(1, x^{2t}), (\infty, x^a)\},\ \{(x^a, x^{a+2t}), (\infty, 1)\}, \tag{6.1}$$

and let the other initial blocks

$$\{(1, x^{2t}), (x^a, x^{a+2t})\} \oplus (x^2, x^4, \ldots, x^{2t-2}), \tag{6.2}$$

be retained as they are. Further let us repeat the whole set of initial blocks (5.2), i.e.,

$$\{(1, x^{2t}), (x^a, x^{a+2t})\} \oplus (1, x^2, x^4, \ldots, x^{2t-2}). \tag{6.3}$$

We shall now use theorem (2), to show that the half-blocks in (6.1), (6.2), (6.3) when developed give the BIB design

$$v_0 = 4t+2,\ b_0 = 2(2t+1)(4t+1),\ r_0 = 2(4t+1),\ k_0 = 2,\ \lambda_0 = 2. \tag{6.4}$$

First note that apart from the two half-blocks (∞, x^a), $(\infty, 1)$ each half block of (5.2) is included twice in (6.1), (6.2) and (6.3) taken together. Hence from what has been proved in section 5, the differences arising from the half-blocks in (6.1), (6.2), (6.3), (after deletion of ∞) are symmetrically repeated twice. It is also easy to check that the condition (iii) of theorem 2 is also satisfied. This proves the required result.

We shall next use the same theorem to prove that the blocks in (6.1), (6.2), (6.3), (disregarding half-blocks) when developed lead to the BIB design

$$v^* = 4t+2,\ b^* = (2t+1)(4t+1),\ r^* = 2(4t+1),\ k^* = 4,\ \lambda^* = 6 \tag{6.5}$$

Comparing with the blocks (5.2), and disregarding ∞, we see that every pair of objects in (5.2), is repeated in (6.2), (6.3) taken together except that the pair x^{2t},

$x^{\alpha+2t}$ in the first case is replaced by the pair 1, x^{α} in the second case. Since $x^{2t}=-1$, the differences $\pm x^{2t}(x^{\alpha}-1)$ arising from x^{2t}, $x^{\alpha+2t}$ are the same as the differences $\pm(x^{\alpha}-1)$ arising from $(x^{\alpha}, 1)$. Also the pairs in (6.3) are the same as in (5.2). Hence it follows as in section 5 that the differences arising from the blocks obtained from (6.2), (6.3), (6.4), after the deletion of ∞, are symmetrically repeated six times. The condition (iii) of Theorem 2 is also easily checked. This proves the statement made above.

Taking together the two results proved we see that when the initial blocks (6.2), (6.3), (6.4) are developed leaving the half-blocks intact, and ∞ unchanged, we get a tournament design belonging to the series (C).

In particular we get the solutions for $u=6$, 10, 14, 18, 26, 30, 38, 42, 50. If $v \leq 50$, this leaves only the values 22, 34 and 46 of the form $4t+2$. These will be considered in section 12.

EXAMPLE 1. Let $t=1$, then the required design has parameters $v=6$, $b=15$, $r=10$, $p=2$, $\lambda_1=2$, $\lambda_2=4$. The initial blocks obtained by using Example 1 section 5 are

$$\{(1, 4), (\infty, 2)\}, \{(2, 3), (\infty, 1)\}, \{(1, 4), (2, 3)\}.$$

EXAMPLE 2. Let $t=2$, then the required design has parameters $v=10$, $b=45$, $r=18$, $p=2$, $\lambda_1=2$, $\lambda_2=4$. The initial blocks obtained by using Example 2 section 5 are

$$\{(1, x^4), (\infty, x)\}, \{(x, x^5), (\infty, 1)\}, \{(1, x^4), (x, x^5)\},$$

and the block

$$\{(x^2, x^5), (x^3, x^7)\}$$

repeated twice. Here x is an element of $GF(3^2)$, with the minimum $x^2+x+2=0$.

EXAMPLE 3. Let $t=2$. The initial blocks of the design with parameters $v=14$, $b=91$, $r=26$, $p=2$, $\lambda_1=2$, $\lambda_2=4$, are

$$\{(1, 12), (\infty, 8)\}, \{(8, 5), (\infty, 1)\}, \{(1, 12), (8, 5)\},$$

and the blocks

$$\{(4, 9), (6, 7)\}, \{(3, 10), (11, 2)\}$$

each taken twice.

7. The Method of Composition for Constructing Tournament Designs

Bose and Shrikhande [5] developed the method of composition for constructing BIB designs. This can be adapted for constructing tournament designs. The method depends on the use of pairwise balanced designs of index unity which were first introduced by Bose and Shrikhande [4] as auxiliary designs useful for the construction of mutually orthogonal Latin squares of nonprime power orders, especially $4t+2$.

An arrangement of v objects in b sets is called a pairwise balanced design of index g and type $(v; k_1, k_2, \ldots, k_m)$ if each block contains either k_1, k_2 . . . or k_m distinct objects which are all distinct $(k_i \leqq v, k_i \neq k_j)$, and every pair of distinct objects occurs in exactly g blocks of the design.

Now suppose there exists a pairwise balanced design D of index g and type $(v^*; k_1^*, k_2^*, \ldots k_m^*)$, with b^* blocks. Let the number of blocks with exactly k_i^* treatments be b_i^*. Then clearly

$$b^*=\sum_{i=1}^{m} b_i^*, \; gv(v-1)=\sum_{i=1}^{m} b_i^* \, k_i^*(k_i^*-1). \qquad (7.1)$$

Also suppose there exist m tournament designs T_i with parameters

$$v_i=k_i, \; b_i, \; r_i=n(v_i-1), \; p_i=p, \; \lambda_{1i}=n(p-1), \; \lambda_{2i}=np, \qquad (7.2)$$

$(i=1, 2, \ldots, m)$, then we can construct a tournament design T with parameters

$$v=v^*, \; b=\sum_{i=1}^{m} b_i b_i^*, \; r=gn(v-1),$$

$$p, \; \lambda_1=gn(p-1), \; \lambda_2=gnp. \qquad (7.3)$$

The objects of the design T will be the same as the objects of D. Let B be a block of D containing k_i objects. We now obtain b_i blocks of T by writing down the b_i blocks of design T_i, the objects being the objects occurring in B. Then among the b_i blocks of T which correspond to B, every pair of objects occurring together in B, will occur in $g\lambda_{1i}$ half-blocks and $g(\lambda_{1i}+\lambda_{2i})$ blocks. We now write down the b_i blocks of T corresponding to each of the b_i^* blocks of D which are of size k_i, obtaining altogether $b_i b_i^*$ blocks. Repeating this for $i=1, 2, \ldots, m$ we get altogether $\sum_{i=1}^{m} b_i b_i^*$ blocks, in which every pair of objects from D, occurs gnp times in half-blocks and $gn(2p-1)$ times in blocks. We thus get the tournament design with parameters (7.3). The case $g=1$ is the most useful.

8. Designs Belonging to the Series (D), When $t \equiv 1 \pmod 3$

Consider the series (D) of bridge tournament designs, when $t=3u+1$. The parameters become

$$v=12u+4, \; b=3(3u+1)(4u+1),$$

$$r=3(4u+1), \; p=2, \; \lambda_1=1, \; \lambda_2=2. \qquad (8.1)$$

In particular the design S_4 with $u=0$ exists if a, b, c, d be the objects. Then the design has the parameters

$$v=4, \; b=3, \; r=3, \; p=2, \; \lambda_1=1, \; \lambda_2=2, \qquad (8.2)$$

and the blocks are

$$\{(a, b), (c, d)\}, \{(a, c), (b, d)\}, \{(a, d), (b, c)\}. \quad (8.3)$$

Now consider the BIB design with parameters

$$v^* = 12u + 4,\ b^* = (3u + 1)(4u + 1),$$

$$r^* = (4u + 1),\ k^* = 4,\ \lambda^* = 1. \quad (8.4)$$

Note that a BIB design with $\lambda^* = 1$ is a special type pairwise balanced design of index unity, where the blocks are all of one type. Taking into account Mann's Lemma given in section 5, a solution to (8.4) can always be found by the method given by Bose in (1), when $4u + 1$ is a prime power. Hanani [8] has shown that a solution exists for all values of u.

If we use the method of composition taking (8.4) as D, and (8.2) as T_1, we get the solution for (8.1).

EXAMPLE 1. Let $u = 1$. The required design has the parameters $v = 16$, $b = 60$, $r = 15$, $p = 2$, $\lambda_1 = 1$, $\lambda_2 = 2$. The corresponding D has initial blocks (cf. [1])

$$(1_1, 4_1, 2_2, 3_2), (1_2, 4_2, 2_3, 3_3), (1_3, 4_3, 2_1, 3_1), (\infty, 0_1, 0_2, 0_3),$$

which have to be developed (mod 5), keeping ∞ and the subscripts invariant. Each initial block gives three initial blocks for the required design. Thus the initial blocks corresponding to $(1_1, 4_1, 2_2, 3_2)$ are

$$\{(1_1, 4_1), (2_2, 3_2)\}, \{(1_1, 2_2), (4_1, 3_2)\}, \{(1_1, 3_2), (4_1, 2_2)\}.$$

In the same way using solutions for (8.4) given in (1), we get the bridge tournament designs belonging to the series (D) for $v = 28$ and 40.

9. Designs Belonging to the Series (D), When $t \equiv 0$ (Mod 5) or 1 (Mod 5)

A solution for the bridge tournament design with parameters

$$v = 5,\ b = 5,\ r = 4,\ p = 2,\ \lambda_1 = 1,\ \lambda_2 = 4, \quad (9.1)$$

has already been given in Example 1, section 5. Now suppose a solution for the BIB design

$$v_0 = 4t + 1,\ b_0 = \frac{t(4t + 1)}{5},\ r_0 = t,\ k_0 = 5,\ \lambda_0 = 1, \quad (9.2)$$

is known. If we delete one particular treatment from all the blocks we get a pairwise balanced design D of type $(4t;\ 4,\ 5)$ with t blocks of size 4, and $4t(t-1)/5$ blocks of size 5. Now we use the method of composition taking for T_1 the design (8.2) and for (T_2) the design (9.1). Then we obtain a solution for the bridge tournament design

$$v = 4t,\ b = t(4t - 1),\ r = 4t - 1,\ p = 2,\ \lambda_1 = 1,\ \lambda_2 = 2.$$

Hence using known solutions from (1), for the BIB designs

(i) $v_0 = 21$, $b_0 = 21$, $r_0 = 5$, $k_0 = 5$, $\lambda_0 = 1$,
(ii) $v_0 = 41$, $b_0 = 82$, $r_0 = 10$, $k_0 = 5$, $\lambda_0 = 1$,
(iii) $v_0 = 25$, $b_0 = 30$, $r_0 = 6$, $k_0 = 5$, $\lambda_0 = 1$,
(iv) $v_0 = 45$, $b_0 = 99$, $r_0 = 11$, $k_0 = 5$, $\lambda_0 = 1$,

we get solutions for bridge tournament designs of the series (D) when $v = 20, 40, 24, 44$. Hanani has shown [8, 9] that a solution for (9.2) always exists when $t \equiv 0$ (mod 5) or 1 (mod 5). Hence under the same conditions, a solution for a bridge tournament design belonging to series (D) always exists.

10. Some Pairwise Balanced Designs of Index Unity Obtained by Adjunction

We have already seen how the method of composition enabled us to obtain solutions of bridge tournament designs with the help of suitable pairwise balanced designs of index unity. Here we shall describe a very useful method of deriving such designs, which will in the sequel be used for the construction of bridge tournament designs.

A BIB design is said to be resolvable if the blocks can be grouped into sets (called replications) such that each object occurs exactly once in each replication. Suppose we have a resolvable BIB design with parameters v^*, b^*, r^*, k^*, λ^*. Let us take c new treatments $\theta_1, \theta_2, \ldots, \theta_c$ $(1 \leq c \leq r)$. To each block of the ith replication add the treatment θ_i, and in case $c > 1$, add a new block $(\theta_1, \theta_2, \ldots, \theta_c)$. We then get a pairwise balanced design of index unity with $v = v^* + c$ objects. Several cases have to be considered separately.

(a) If $c = 1$, the new design obtained is of the type $(v^* + 1;\ k^* + 1,\ k^*)$, with v^*/k^* of size $k^* + 1$ and $b^* - (v^*/k^*)$ blocks of size k^*.

(b) If $c > 1$ and $c \neq k^*$, $k^* + 1$ or r^* then the new design is of the type $(v^* + c;\ k^* + 1, k^*, c)$ with cv^*/k^* blocks of size $k^* + 1$, $b^* - (cv^*/k^*)$ blocks of size k^* and one block of size c.

(c) If $c = k^* < r^*$ then the new design is of the type $(v^* + c;\ k^* + 1,\ k^*)$ with v^* blocks of size $k^* + 1$ and $b^* - v^* + 1$ blocks of size k^*.

(d) If $c = k^* + 1 < r^*$, then the new design is of the type $(v^* + c,\ k^* + 1,\ k^*)$ with $1 + \{(k^* + 1)v^*/k^*\}$ blocks of size $k + 1$ and $b - \{(k^* + 1)v^*/k^*\}$ blocks of size k^*.

(e) If $c = r^* > k^* + 1$ then the new design is of the type $(v^* + c,\ k^* + 1,\ c)$ with b^* blocks of size $k^* + 1$ and one block of size $c = r^*$.

Three resolvable BIB designs which we shall use in this manner together with their solutions are given below [see Bose, Shrikhande, and Bhattacharya [6], table III, p. 171].

Parameters	Solution
(1) $v^*=28$, $b^*=63$, $r^*=9$, $k^*=4$, $\lambda^*=1$	One replication is given by $(01_1, 02_1, 10_2, 20_2)$, $(21_1, 12_1, 22_2, 11_2)$ $(01_2, 02_2, 10_3, 20_3)$, $(21_2, 12_2, 22_3, 11_3)$ $(01_3, 02_3, 10_1, 20_1)$, $(21_3, 12_3, 22_1, 11_1)$ $(00_1, 00_2, 00_3, \infty)$. Other replications are obtained by developing (mod 3, 3).
(2) $v=40$, $b=130$, $r=13$, $k=4$, $\lambda=1$	One replication is given by $(1_1, 12_1, 8_2, 5_2)$, $(4_1, 9_1, 6_2, 7_2)$, $(3_1, 10_1, 11_2, 2_2)$ $(1_2, 12_2, 8_3, 5_3)$, $(4_2, 9_2, 6_3, 7_3)$, $(3_2, 10_2, 11_3, 2_3)$ $(1_3, 12_3, 8_1, 5_1)$, $(4_3, 9_3, 6_1, 7_1)$, $(3_3, 10_3, 11_1, 2_1)$ $(\infty, 0_1, 0_2, 0_3)$. The other replications are obtained by developing (mod 13).
(3) $v=15$, $b=35$, $r=1$, $k=3$, $\lambda=1$	One replication is given by $(1_1, 2_1, 4_1)$, $(3_1, 1_2, 5_2)$, $(6_1, 2_2, 3_2)$ $(5_1, 4_2, 6_2)$, $(0_1, 0_2, \infty)$. The other replications are obtained by developing (mod 7).

11. Designs Belonging to the Series (B), for $t=5$, 8 and 11

When $t=5$, 8 or 11 then $4t+1$ is not a prime power. Hence the method of section 4 fails. A solution for these cases can however be obtained by using the method of composition.

(a) Let $t=5$. The required design has the parameters

$$v=21,\ b=105,\ r=20,\ \lambda_1=1,\ \lambda_2=2. \qquad (11.1)$$

The solution follows from the method of composition by using for D the BIB design

$$v^*=21,\ b^*=21,\ r^*=5,\ k^*=5,\ \lambda^*=1. \qquad (11.2)$$

and for T_1 the design S_3 with parameters (9.1) with the solution given in section 5, Example 1. The solution for (11.2) is found by developing mod 21, the initial block [cf. [6], p. 170]

$$(0, 1, 4, 14, 16). \qquad (11.3)$$

(b) Let $t=8$. The required design has the parameters (10.3)

$$v=33,\ b=264,\ r=32,\ p=2,\ \lambda_1=1,\ \lambda_2=2. \qquad (11.4)$$

We start from a resolvable solution of the BIB design

$$v^*=28,\ b^*=63,\ r^*=9,\ k^*=4,\ \lambda^*=1. \qquad (11.5)$$

given in section 10. By adjoining 5 new objects we get a pairwise balanced design D of index unity and type (33; 5, 4) with 36 blocks of size 5 and 28 blocks of size 4. The required design is now obtained by applying the method of composition, using D and taking for T_1 and T_2 the designs S_5 and S_4 with parameters (9.1) and (8.2).

(c) Let $t=11$. The required design has parameters

$$v=45,\ b=495,\ r=44,\ p=2,\ \lambda_1=1,\ \lambda_2=2. \qquad (11.6)$$

A solution to this can be obtained from the method of composition by using for D the BIB design

$$v^*=45,\ b^*=99,\ r^*=11,\ k^*=5,\ \lambda^*=1, \qquad (11.7)$$

and for T_1 the design S_5 with parameters (9.1). For a solution to D see [1], p. 389.

12. Designs Belonging to the Series (C), for $t=5$, 8, and 11

Since $4t+1$ is not a prime power when $t=5$, 8 or 11, the method of section 6 fails. We can however use the method of composition to obtain the corresponding designs.

(a) Let $t=5$. The required design has the parameters

$$v=22,\ b=231,\ r=42,\ p=2,\ \lambda_1=2,\ \lambda_2=4. \qquad (12.1)$$

We start from a resolvable solution of the BIB design

$$v^*=15,\ b^*=35,\ r^*=7,\ k^*=4,\ \lambda^*=1 \qquad (12.2)$$

given in section 10. By adjoining 7 new objects we get a pairwise balanced design of index unity and type (22; 4, 7).

Let S_4^* and S_7^* be bridge tournament designs with parameters given by (12.3) and (12.4):

$$v=4,\ b=6,\ r=6,\ p=2,\ \lambda_1=2,\ \lambda_2=4. \qquad (12.3)$$

$$v=7,\ b_2=21,\ r_2=12,\ p=2,\ \lambda_1=2,\ \lambda_2=4. \qquad (12.4)$$

Note that S_4^* is not a minimal design. The solution for S_4^* is simply obtained by duplicating the blocks (8.3). The solution for S_7^* is given in section 4, Example 1.

The required design (12.1) is now obtained by applying the method of composition using D and taking S_4^* and S_7^* for T_1 and T_2.

(b) Let $t=8$. The required design has the parameters

$$v=34,\ b=561,\ r=66,\ p=2,\ \lambda_1=2,\ \lambda_2=4. \qquad (12.5)$$

We start from the resolvable solution of the BIB design

$$v^*=28,\ b^*=63,\ r^*=9,\ k^*=4,\ \lambda^*=1,$$

given in section 10. By adjoining six new objects we get a pairwise balanced design D of index unity and type (34; 4, 5, 6) with 21 blocks of size 4, 42 blocks of size 5 and one block of size 6.

Let S_6^* be the bridge tournament design with parameters

$$v=6,\ b=15,\ r=10,\ p=2,\ \lambda_1=2,\ \lambda_2=4 \quad (12.6)$$

the solution for which is given in section 6, example (1). Also let S_5^* be the design with parameters

$$v=5,\ b=10,\ r=8,\ p=2,\ \lambda_1=2,\ \lambda_2=8 \quad (12.7)$$

the solution for which is obtained by duplicating the solution for (9.1).

The required solution for (12.5) not follows by applying the method of composition using D, and the designs S_4^*, S_5^*, and S_6^* for T_1, T_2, and T_3. Note that the number of blocks obtained is

$$21(6)+42(10)+1(15)=561$$

which checks.

(c) Let $t=11$. The required design has the parameters

$$v=46,\quad b=1035,\quad r=90,\quad p=2,\quad \lambda_1=2,\quad \lambda_2=4. \quad (12.8)$$

We start from the resolvable solution of the BIB design

$$v^*=40,\quad b^*=130,\quad r^*=13,\quad k^*=4,\quad \lambda^*=1 \quad (12.9)$$

given in section 10, and obtain from it a pairwise balanced design D of index unity and type (46; 4, 5, 6) with 70 blocks of size 4, 60 blocks of size 5 and one block of size 6. Applying the method of composition using D, and the designs S_4^*, S_5^*, and S_6^* as T_1, T_2, T_3 we get the required solution for (12.8).

13. Designs Belonging to Series (D), for $t=2$, 3, 8, 9, and 12

(a) Let $t=2$. The required design has the parameters

$$v=8,\quad b=14,\quad r=7,\quad p=2,\quad \lambda_1=1,\quad \lambda_2=2. \quad (13.1)$$

Let us associate one object to each element of $GF(7)$ and adjoin another object $\propto$. Then a solution to the required design is obtained by developing mod 7 the initial blocks

$$\{(0, 1), (4, 2)\},\qquad \{(1, 4), (2, \propto)\}. \quad (13.2)$$

The proof follows by observing that from Theorem (2), the two initial blocks in (13.2), disregarding half-blocks, provide a solution of the BIB design [see Bose [2], p. 30]

$$v^*=8,\quad b^*=14,\quad r^*=7,\quad k^*=4,\quad \lambda^*=3,$$

and the half-blocks provide a solution of the BIB design

$$v^*=8,\quad b^*=28,\quad r^*=7,\quad k^*=2,\quad \lambda^*=1.$$

(b) Let $t=3$. The required design has the parameters

$$v=12,\quad b=33,\quad r=11,\quad p=2,\quad \lambda_1=1,\quad \lambda_2=2. \quad (13.3)$$

Let us associate one object to each element of $GF(11)$, and adjoin another object $\propto$. Then a solution of the required design is obtained by developing (mod 11) the initial blocks

$$\{(0, 1), (3, 7)\},\quad \{(4, 9), (2, 10)\},\quad \{(\propto, 5), (6, 8)\}. \quad (13.4)$$

If we disregard the half-blocks, then the initial blocks (13.4) provide a solution of the BIB design

$$v^*=12,\quad b^*=33,\quad r^*=11,\quad k^*=4,\quad \lambda^*=3. \quad (13.5)$$

This solution was given by Rao [12]. Also the half-blocks in (13.4) provide a solution of the BIB design

$$v^*=12,\quad b^*=66,\quad r^*=22,\quad k^*=2,\quad \lambda^*=1. \quad (13.6)$$

(c) Let $t=8$ or 9. The two required designs have the parameters

$$v=32,\quad b=248,\quad r=31,\quad p=2,\quad \lambda_1=1,\quad \lambda_2=2 \quad (13.7)$$

$$v=36,\quad b=315,\quad r=35,\quad p=2,\quad \lambda_1=1,\quad \lambda_2=2. \quad (13.8)$$

Starting from the resolvable solution of the BIB design with parameters

$$v^*=28,\ b^*=63,\ r^*=9,\ k^*=4,\ \lambda^*=1,$$

we can by adjoining x treatments ($x=4$, 8), and a new block of size x obtain pairwise balanced designs D_1 and D_2 of index unity and types (32; 4, 5) and (36; 4, 5, 8).

The solution of (13.7) follows by applying the method of composition using D_1 and the designs S_4 and S_5, with parameters (8.2) and (9.1), as T_1 and T_2.

Again let S_8 be the design with parameters (13.1). Then a solution of (13.8) follows by applying the method of composition using D_2 and the designs S_4, S_5, and S_8 for T_1, T_2, and T_3.

(d) Let $t=12$. The required design has the parameters

$$v=48,\ b=564,\ r=47,\ p=2,\ \lambda_1=1,\ \lambda_2=2. \tag{13.9}$$

We start from the resolvable solution of the BIB design

$$v=40,\ b=130,\ r=13,\ k=4,\ \lambda=1,$$

given in section 10, and derive from it a pairwise balanced design D of index unity and type (48; 4, 5, 8), by adjoining 8 new treatments.

We can now apply the method of composition using D together with the designs S_4, S_5, and S_8 as T_1, T_2, T_3 to obtain the solution of (13.9).

14. Designs Belonging to the Series (A), for $t=3$, 8, and 9 and the Use of Group Divisible Designs

(a) Let us first consider the case $t=8$. Then the required design has the parameters

$$v=35,\ b=595,\ r=68,\ p=2,\ \lambda_1=2,\ \lambda_2=4. \tag{14.1}$$

We start from the resolvable solution of the BIB design

$$v^*=28,\ b^*=63,\ r^*=9,\ k^*=4,\ \lambda^*=1,$$

given in section 10, and obtain from it a pairwise balanced design D of index unity and type (35; 4, 5, 7) with 14 blocks of size 4, 49 blocks of size 5, and one block of size 7.

Let S_4^* and S_5^* be as in section 12, and let S_7^* be the bridge tournament design with parameters

$$v=7,\ b=21,\ r=12,\ p=2,\ \lambda_1=2,\ \lambda_2=1, \tag{14.2}$$

the solution for which is given in section 4, Example 1.

The required solution for (14.1) is then obtained by applying the method of composition using D together with the designs S_4^*, S_5^* and S_7^* for T_1, T_2, T_3. Note that the number of blocks obtained is

$$14(6)+49(10)+21(1)=595.$$

(b) We have now obtained all minimal bridge tournament designs for $v\leq 50$, except the following two designs

$$v=39,\ b=741,\ r=76,\ p=2,\ \lambda_1=2,\ \lambda_2=4, \tag{14.3}$$

$$v=15,\ b=105,\ r=28,\ p=2,\ \lambda_1=2,\ \lambda_2=4, \tag{14.4}$$

both belonging to the series (A). We shall use group divisible (GD) designs for constructing the solution of these designs. For the combinatorial properties and the methods of construction for these designs refer to Bose and Connor [3] and Bose, Shrikhande, and Bhattacharya [6].

Given $v_0=m_0n_0$ objects divided into m_0 groups each with n_0 treatments, a GD design with parameters

$$v_0,\ b_0,\ r_0,\ k_0,\ m_0,\ n_0,\ \lambda_{10},\ \lambda_{20}, \tag{14.5}$$

is an arrangement of the objects in b_0 blocks each of size k_0, such that any two objects belonging to the same group occur together in λ_{10} blocks, and any two objects belonging to different groups occur together in λ_{20} blocks.

(b) For a solution of (14.3) we start from the GD design with parameters

$$v_0=32,\ b_0=64,\ r_0=8,\ k_0=4,$$

$$m_0=4,\ n_0=8,\ \lambda_{10}=0,\ \lambda_{20}=1. \tag{14.6}$$

A method of obtaining a resolvable solution of this design is given in [6], table VII, p. 186. Let us take 7 new treatments $32+i (i=1, 2, \ldots, 7)$. To each block of the ith replication add the treatment $32+i$. Also take as blocks the groups, and also add a new block consisting of the 7 new treatments. We then get a pairwise balanced design D of index unity and type (39; 4, 5, 7, 8) with 8, 56, 1 and 4 blocks of size 4, 5, 7 and 8 respectively.

Let S_4^*, S_5^*, be as in section 12, let S_7^* be the design with parameters (14.2), and let S_8^* be the design with parameters

$$v=8,\ b=28,\ r=14,\ p=2,\ \lambda_1=1,\ \lambda_2=2,$$

obtained by duplicating the design (13.1) whose solution is given in section 13(a).

We now get the required solution for (14.3) by applying the method of composition using (D), together with the designs S_4^*, S_5^*, S_7^*, and S_8^* as T_1, T_2, T_3, T_4. Note that the number of blocks obtained is

$$8(6)+56(10)+1(21)+4(28)=741.$$

(c) For a solution of (14.3) we have to start out from the GD design with parameters

$$v=15,\ b=30,\ r=8,\ k=4,\ m=3,\ n=5,\ \lambda_1=1,\ \lambda_2=2 \tag{14.6}$$

[see Bose, Shrikhande, and Bhattacharya [6], table VI, No. (17), p. 178]. The treatments can be identified with pairs (c, d) where c belongs to $GF(5)$ and d to $GF(3)$. Thus $(c_1, d_1)+(c_2, d_2)=(c, d)$ where $c_1+c_2\equiv c \pmod 5$, $d_1+d_2\equiv d \pmod 3$. The three

groups are

$$\begin{array}{ll} \text{Group I} & 00, 10, 20, 30, 40; \\ \text{Group II} & 01, 11, 21, 31, 41; \\ \text{Group III} & 02, 12, 22, 32, 42. \end{array} \tag{14.7}$$

The blocks of (15.6) are obtained by developing the initial blocks

$$(00, 40, 21, 22), \quad (00, 20, 11, 31, 41), \quad (\text{mod } 5, 3). \tag{14.8}$$

If to the 30 blocks constituting the solution of (15.6), we add the three groups as blocks, we get a pairwise balanced design D of index 2 and type (15; 4, 5) with 30 blocks of size 4 and 3 blocks of size 5. We now use the method of composition employing this design, and taking for T_1 and T_2 the designs S_4 and S_5 with parameters (8.2), (9.1). We then get the required solution for (14.3). Note that the number of blocks obtained is

$$30(3)+3(5)=105.$$

(Paper 69B4–162)

15. References

[1] R. C. Bose, On the construction of balanced incomplete block designs, Ann. Eugen. **9**, 353–399 (1939).

[2] R. C. Bose, On some new series of balanced incomplete block designs, Bull. Cal. Math. Soc. **34**, 17–31 (1942).

[3] R. C. Bose and W. S. Conner, Combinatorial properties of group divisible incomplete block designs, Ann. Math. Stat. **23**, 367–383 (1952).

[4] R. C. Bose and S. S. Shrikhande, On the construction of sets of mutually orthogonal Latin squares and the falsity of a conjecture of Euler, Trans. Amer. Math. Soc. **95**, 191–209 (1960).

[5] R. C. Bose and S. S. Shrikhande, On the composition of balanced incomplete block designs, Can. J. Math. 177–188 (1960).

[6] R. C. Bose, S. S. Shrikhande, and K. N. Bhattacharya, On the construction of group divisible incomplete block designs, Ann. Math. Stat. **24**, 167–195 (1953).

[7] Lewis Caroll, On the scheduling of lawn tennis tournaments, Complete works of Lewis Caroll, Modern Library.

[8] Haim Hanani, The existence and construction of balanced incomplete block designs, Ann. Math. **32**, 361–386 (1961).

[9] Haim Hanani, A balanced incomplete block design, Ann. Math. Stat. **36**, 711 (1965).

[10] M. Kraitchik, Mathematical Recreations (W. W. Norton and Co., Inc., New York, 1942).

[11] H. B. Mann, Analysis and Design of Experiments (Dover Publications, Inc., New York, 1949).

[12] C. R. Rao, A study of BIB designs with replications 11 to 15, Sankhya, series A, **23**, 117–127 (1961).

[13] Francis Scheid, A tournament problem, Amer. Math. Monthly **67**, 39–41 (1960).

[14] C. C. Yalavigi, A tournament problem, Math. Student **31**, 51–64 (1963).

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 69B, No. 4, October–December 1965

The Condition of Certain Matrices*

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(September 8, 1965)

By reversing the usual direction of application, a common procedure for solving integral equations numerically is used to obtain the asymptotic P-condition numbers of two well-known test matrices.

Key Words: Asymptotic P-condition, integral equations, test matrices.

Todd [1][1] has recently suggested the matrix $A_{17} = (|i-j|)$, $1 \leq i, j \leq n$, as an addition to the well-known collection of test matrices [2]. The P-condition numbers of the matrices are used as a measure of their difficulty for numerical purposes. Where the condition numbers are not explicitly known, the asymptotic behavior in n is given. Lehmer's matrix A_7

$$a_{ij} = i/j \qquad i \leq j$$
$$= j/i \qquad j < i$$

is exceptional in that the correct order in n is not known. A simple idea will allow us to obtain the asymptotic condition number of A_{17} and the correct order for A_7.

Hilbert's first method for integral equations [3] approximates the eigenvalues of the kernel $K(x, y)$, $0 \leq x, y \leq 1$, by those of the matrix

$$\frac{1}{n}\left(K\left(\frac{i}{n}, \frac{j}{n}\right)\right).$$

If K is bounded and Riemann integrable, then the eigenvalues of the matrices tend to those of the integral equation as n tends to ∞. We reverse this procedure. We wish to estimate the behavior of the eigenvalues of a set of matrices as n tends to ∞. If we can regard them as arising from the application of Hilbert's first method to a fixed kernel, then we may hope for an asymptotic result.

To estimate the largest eigenvalue of A_{17}, let us form

$$\frac{1}{n^2}(|i-j|) = \frac{1}{n}\left(\left|\frac{i}{n} - \frac{j}{n}\right|\right).$$

We regard them as arising from the approximation of the kernel

$$K(x, y) = |x - y|.$$

A simple computation gives the largest eigenvalue of K as

$$\lambda_1 = \tfrac{1}{2} z_0^{-2}$$

where z_0 is the unique real root of $\coth z = z$. This equation has been studied [4] and z_0 is approximately $z_0 = 1.9967864$. We conclude that the largest eigenvalue of A_{17} is asymptotically

$$\lambda_1 \sim \tfrac{1}{2} z_0^{-2} n^2.$$

It is easy to estimate the accuracy of the approximation using the bounds of [5] but we shall not go into this.

We need the reciprocal of the eigenvalue of A_{17} smallest in modulus. It is obtained as the largest eigenvalue of the inverse matrix.

Let us introduce the matrices

$$M = -2A_{17}^{-1},$$

$$N = \begin{Vmatrix} 1, -1 & & & \\ -1, 2, -1 & & & \\ & \ddots & \ddots & \ddots \\ & & -1, 2, -1 & \\ & & & -1, 1 \end{Vmatrix}$$

and Q where $\begin{cases} q_{11} = q_{1n} = q_{n1} = q_{nn} = \dfrac{1}{n-1} \\ q_{ij} = 0 \text{ otherwise.} \end{cases}$

*This work was supported by the United States Atomic Energy Commission. Reproduction in whole or in part is permitted for any purpose of the U.S. Government.

[1] Figures in brackets indicate the literature references at the end of this paper.

It is readily verified that

$$A_{17}^{-1} = \tfrac{1}{2}(Q - N)$$

or

$$M + Q = N.$$

Q is obviously a positive semidefinite matrix. By a well-known inequality [6, p. 73],

$$\lambda_1(N) = \lambda_1(M + Q) \geq \lambda_1(M).$$

Rutherford [7] has shown that the eigenvalues of N are

$$4 \cos^2 \frac{i\pi}{2n} \qquad i = 1, 2, \ldots, n.$$

and the eigenvector associated with $\lambda_1(N)$ is

$$x_j = \sin \frac{j\pi}{n} - \sin \frac{(j-1)\pi}{n} \qquad j = 1, \ldots, n.$$

The Rayleigh quotient furnishes a lower bound to $\lambda_1(M)$. A convenient approximate eigenvector is that associated with $\lambda_1(N)$. For this vector

$$\lambda_R(M) = \frac{(x, Mx)}{(x, x)} = \lambda_1(N) - \frac{(x_1 + x_n)^2}{(n-1)(x, x)}.$$

A little algebraic manipulation gives

$$\lambda_R(M) = \lambda_1(N) - \frac{8 \sin^2 \dfrac{\pi}{n}}{n(n-1)\lambda_1(N)}.$$

Thus

$$\lambda_R(M) \leq \lambda_1(M) \leq \lambda_1(N)$$

and we see

$$\lambda_1(M) = \lambda_1(N) + 0(n^{-4}).$$

From this

$$\left| \frac{1}{\lambda_n(A_{17})} \right| = 2 \cos^2 \frac{\pi}{2n} + 0(n^{-4})$$

and finally

$$P(A_{17}) \sim z_0^{-2} n^2 \cos^2 \frac{\pi}{2n}.$$

The same methods applied to the kernel

$$K(x, y) = x/y \qquad x \leq y$$

$$y/x \qquad y < x$$

show that for A_7, $\lambda_1 = 0(1)$. The inverse is explicitly

$$\frac{4i^3}{4i^2 - 1} \qquad i = j,\ i < n$$

$$\frac{n^2}{2n-1} \qquad i = j = n$$

$$-\frac{i(i+1)}{2i+1} \qquad |i-j| = 1$$

$$0 \qquad |i-j| > 1.$$

Gerschgorin's theorem immediately gives $\left| \dfrac{1}{\lambda_n} \right| = 0(n)$. Todd and Newman comment that $P(A_7) \geq n$. From this we conclude that $P(A_7) \sim cn$ where c is a constant.

References

[1] J. Todd, The Problem of Error in Digital Computation, Error in Digital Computation, L. B. Rall, ed. (University of Wisconsin Press, 1965).

[2] M. Newman and J. Todd, The Evaluation of Matrix Inversion Programs, J.S.I.A.M., **6**, 466 (1958).

[3] D. Hilbert, Grundzüge einer allgemeinen Theorie der linearen Integralgleichungen, Erste Mitteillung, Nachr. Ges. Wiss. Göttingen, pp. 49–91 (1904).

[4] A. Fletcher, J. C. P. Miller, and L. Rosenhead, An Index of Mathematical Tables, London–New York, 1946.

[5] H. Wielandt, Error Bounds for Eigenvalues of Symmetric Integral Equations, Proceedings of Symposia in Applied Mathematics, Vol. **VI**, (McGraw-Hill Book Co., New York, N.Y., 1956).

[6] E. Beckenbach and R. Bellman, Inequalities (Springer-Verlag, Berlin, 1961).

[7] D. E. Rutherford, Some continuant determinants arising in physics and chemistry, Proc. Roy. Soc. Edinburgh **62A**, 229–236.

(Paper 69B4–163)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 69B, No. 4, October–December 1965

Some Number-Theoretic Calculations

K. E. Kloss

(September 29, 1965)

An account is given of several number-theoretic computations carried out by the author, some with ranges many times those of any previous published work. The calculations pertain to (1) long sequences of consecutive composite numbers, (2) Fermat quotients, (3) Wilson quotients, (4) generalized Wilson quotients, (5) Pell's equation, (6) the partition function, (7) a conjecture of Feit and Thompson, and (8) unique factorization quadratic domains.

Key words: Numbers, theory of, primes.

The purpose of this note is to enumerate some number-theoretic calculations carried out by the author in the past four years. By so doing, we hope to prevent needless repetition of the calculations elsewhere. We expect to describe most of the computations in greater detail in later articles; our intention here is just to offer a convenient summary. Most of the calculations were done on the NBS PILOT computer, a decimal and hexadecimal machine with a 65-bit word.

The results obtained were the following:

1. Consecutive Composite Numbers. The greatest difference between consecutive primes less than 128,000,000 is 222. It occurs between $p_0 = 122{,}164{,}747$ and $p_0 + 222$.

2. Fermat Quotients. For p an odd prime, the congruence

$$a^{p-1} \equiv 1 \mod p^2$$

is important in the "first case" of Fermat's Last Theorem, for it is known (J. B. Rosser, An additional criterion for the first case of Fermat's last theorem, Bull-AMS **47** (1941), 109–110) that a counterexample to the Theorem, with odd prime exponent p, can exist only if this congruence is satisfied by all primes $a \leq 43$. The following table gives, for all primes $a \leq 43$, all odd prime solutions p of the congruence which are less than the indicated range $R(a)$ of the calculation.

3. Wilson Quotients. The only known solutions of

$$(p-1)! + 1 \equiv 0 \mod p^2$$

are $p = 5$; 13; 563. There are no other solutions $p < 1{,}017{,}000$, but there are some "near" solutions like

$$\{(780{,}886)! + 1\}/780{,}887 \equiv -1 \mod 780{,}887.$$

TABLE 1. *Odd prime solutions of* $a^{p-1} \equiv 1 \mod p^2$

a	$R(a)$	p
2	31,059,000	1,093; 3,511
3	10,752,000	11; 1,006,003
5	5,250,000	20,771; 40,487
7	10,057,000	5; 491,531
11	7,736,000	71
13	5,243,500	7; 863; 1,747,591
17	5,415,900	3; 46,021; 48,947
19	5,583,900	3; 13; 43; 137
23	5,131,970	13; 2,481,757
29	10,431,000	No solutions found.
31	10,450,000	7; 79; 6,451
37	10,309,750	3; 77,867
41	9,500,000	29; 1,025,273
43	5,430,200	5; 103

4. Generalized Wilson Quotients. Let $t(n)$ denote the product of all positive integers less than and relatively prime to n. In the range $3 \leq n < 32{,}000$, the only n for which

$$t(n) \equiv \pm 1 \mod n^2$$

were found to be $n = 5$; 13; 563 (see sec. 3) and

$$n = 5{,}971 = 7 \times 853.$$

5. Pell's Equation. A table was prepared showing, all integers $N < 96{,}562$ for which

$$x^2 - Ny^2 = -1 \qquad (1)$$

has solutions in integers x, y. There is also a table of all integers $N < 96{,}562$ which are the sum of two relatively prime squares and for which (1) is not solvable.

6. Partition Function. Let $p(n)$ denote the number of (unrestricted) partitions of n. Tables of $p(n)$ mod m were calculated for $m = 11^7$ and 13^7 ($n \leq 25{,}000$), and $m = 19^6$, 23^5, 29^2 ($n \leq 1{,}000$).

In addition it was shown that for each prime q in the range $13 \leq q \leq 47$, and for every integer b, there is an integer $a > 0$ such that $p(aq+b) \not\equiv 0 \bmod q$.

7. *A Conjecture of Feit and Thompson.* There are no primes $p < 550{,}800$ such that

$$p^2+p+1 \text{ is a prime and } 3^p \equiv 1 \bmod (p^2+p+1).$$

This is in agreement with the Feit-Thompson conjecture that

$$\left(\frac{p^q-1}{p-1}, \frac{q^p-1}{q-1}\right) = 1$$

for distinct primes p and q. The displayed condition is equivalent to the conjecture for the case $q=3$.

8. *Unique Factorization Domains.* For primes $p \equiv 1 \bmod 4$, let $h(p)$ denote the class number of the integral domain

$$\left\{\frac{a+b\sqrt{p}}{2} : a, b \text{ rational integers of the same parity}\right\}.$$

For $p < 120{,}000$, approximately 80 percent of such integral domains have unique factorization (i.e., have $h(p)=1$). A table of such p yielded this information.

In addition, a table of $h(p)$ for $p < 95{,}000$ was calculated.

The author acknowledges and expresses appreciation for the considerable assistance and cooperation of the PILOT staff, especially William Truitt.

(Paper 169B4-164)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 69B4, No. 4, October–December 1965

Publications of the National Bureau of Standards*

Selected Abstracts

Correlation of successive atomic steps in crystals by relaxation mode analysis, A. D. Franklin, *J. Res. NBS* **69A** (*Phys. and Chem.*), *No. 4, 301–307 (July–Aug. 1965), 70 cents.*
The relaxation mode analysis is used to compute the average value of the cosine of the angle between successive steps of an ion diffusing by a vacancy mechanism on a lattice. The technique is applicable to tracers (self-diffusion) or impurities, on any lattice. The result, given in terms of the eigenvalues and eigenvectors of a secular equation, is suitable for machine computation. Sample computations for self-diffusion on an fcc lattice illustrate the method. It is necessary, in order to do the calculations, to have a lattice of finite size, the boundary of which is chosen either totally reflecting or completely transparent to vacancies. For self-diffusion, the boundary can be centered on the vacancy, and convergence of the computed value with boundary radius is rapid. For impurity diffusion, the boundary must be centered on the impurity, and convergence is much slower.

Distribution function of the end-to-end distances of linear polymers with excluded volume effects, J. Mazur, *J. Res. NBS* **69A** (*Phys. and Chem.*), *No. 4, 355–363 (July–Aug. 1965), 70 cents.*
The distribution function of the absolute values of chain lengths of a polymer molecule which displays the excluded volume effect cannot assume a Gaussian form. This fact follows directly from theoretical considerations based on the application of the Central Limit Theorem to the theory of Markov chains. In order to determine the exact shape of the polymer chain-end distribution function we calculated its various moments taken about the origin, and their dependence on the number of polymer segments, using a Monte Carlo technique for generating polymer chains on a lattice. The results obtained from the extrapolation of various combinations of these moments of the general form

$$\delta_n = \frac{< r_n^p >}{< r_n^{p/2} >^s} - 1 \text{ for } n \to \infty \text{ are used to determine}$$

the shape of the polymer distribution function. It is found that the chain-end distribution function can be approximated by the following form:

$$W(r)dr = \left[\Gamma\left(\frac{3}{t}\right)\right]^{-1} t\alpha^{3/t} r^2 \exp(-\alpha r^t)dr, \text{ with } t = 3.2 \text{ and}$$

α being a parameter, determinable from the average mean square chain-end distances.

Errors in the series-parallel buildup of four-terminal resistors, C. H. Page, *J. Res. NBS* **69C** (*Eng. and Instr.*), *No. 3, 181–189 (July–Sept. 1965), 75 cents.*
The use of n equal resistors (a) in series and (b) in parallel provides an n^2:1 ratio of potentially high accuracy. Such devices are important for extending the use of the national one-ohm standard to the hundred-ohm, and thence to the 10 000-ohm level.
Formulas are derived for the error in the ratio, expressed (a) in terms of design tolerance, and (b) in terms of first-order residual misadjustments which combine to yield the second-order error of the ratio. It seems feasible to construct a 1:100 ohm buildup device with a ratio uncertainty of less than 1 in 10^8.

Theory of coil antennas, T. Padhi, *Radio Sci. J. Res. NBS/USNC–URSI*, **69D,** *No. 7, 977–987 (July 1965), $1.00.*
In this paper, a method is presented by which the distribution of current on some structurally simple coil or multiturn loop antennas may be obtained. The input admittances of unshielded and shielded coils are determined and their operation as receiving elements is considered.

A theorem on the automorphs of a skew-symmetric matrix, M. Newman, *Mich. Math. J.* **12,** *61–63 (1965).*
Let K be an integral non-singular skew-symmetric matrix. It is shown that if a matrix M_0 satisfies

$$M_0 K M_0' \equiv K \pmod{n}$$

then an integral matrix M exists such that $M \equiv M_0 \pmod{n}$ and

$$MKM' = K.$$

On the location of the zeros of some infrapolynomials with prescribed coefficients, J. L. Walsh and O. Shisha, *Pacific J. Math.* **14,** *No. 3, 1103–1109 (1964).*
Some results are given concerning the zeros of infrapolynomials with prescribed coefficients. An application of infrapolynomials to the general theory of the distribution of zeros of rational functions is also given.

On the structure of infrapolynomials with prescribed coefficients, O. Shisha, *Pacific J. Math.* **14,** *No. 3, 1039–1051 (1964).*
The main result of this paper is a theorem (Theorem 5) on the structure of infrapolynomials with prescribed coefficients. It has applications (in this paper and elsewhere) to the study of the geometrical location of the zeros of some infrapolynomials with prescribed coefficients.

On trapped trajectories in Brownian motion, J. L. Jackson and S. R. Coriell, *J. Math. Phys.* **5,** *No. 8, 1075–1078 (Aug. 1964).*
For a Brownian particle moving in the attractive field of a line change, the possibility of trapped trajectories, i.e., trajectories which never depart from the center of attraction, is shown.

Stability of the shape of a solid cylinder growing in a diffusion field, R. L. Parker and S. R. Coriell, *J. Appl. Phys.* **36,** *No. 2, 632–637 (Feb. 1965).*
The stability of the shape of an infinite cylinder undergoing radial growth controlled by diffusion is studied by a method originated by Mullins and Sekerka (MS). It is found that the circular cross section of a cylinder is stable when its radius is below, and unstable when its radius is above a certain radius R_c. This result is analogous to the MS result that a sphere is stable below and unstable above a certain radius R_c, which is seven times the critical radius R^* of nucleation theory. However, in the present case, the ratio R_c/R^* is not equal to seven, but is a function of $S = (c_\infty - c_s)/(C - c_s)$, where c_∞, c_s, and C are the concentrations of the solute at infinity, at the surface of the cylinder, and in the precipitate, respectively. The case of perturbations in the radius along the length of the cylinder is also treated.

A uniqueness theorem for entire functions, R. F. DeMar, *Proc. Am. Math. Soc.* **16,** *No. 1, 69–71 (Feb. 1965).*
Let $K[\Omega]$ denote the class of entire functions f of exponential type whose Borel transforms F are regular on Ω', the complement of a simply connected set Ω. Let $\{\mathscr{L}_n\}$ be a sequence of linear functionals defined on $K[\Omega]$ by $\mathscr{L}_n(f) = (2\pi i)^{-1} \int_\Gamma [W(\zeta)]^n F(\zeta) d\zeta$ for some function W regular on Ω where Γ is a simple contour contained in Ω and enclosing all singularities of F. For such a sequence of functionals, it is shown that $K[\Omega]$ is a uniqueness class for $\{\mathscr{L}_n\}$ (i.e., $f \in K[\Omega]$ and $\mathscr{L}_n(f) = 0$; $n = 0, 1, 2, \ldots$ implies $f = 0$) if and only if W is univalent on Ω. Gelfond has proved the necessity of this condition, but the best previous sufficient condition had the additional hypotheses that Ω contain the origin, $W(0) = 0$, and W map Ω onto a set which is star-shaped with respect to the origin.

On a theorem concerning existence of interpolating functions, R. F. DeMar, *Trans. Am. Math. Soc.* **114,** *No. 1, 23–29 (Jan. 1965).*

If C is an open connected set in the plane, let $K(C)$ denote the class of all entire functions f of exponential type such that the Laplace transform F of f has a continuation regular on C', the complement of C. For a sequence $\{\mathcal{L}_n\}$ of linear functionals having a certain integral representation and a class $K(C)$ for C an open convex set containing the origin and contained in a certain set, in an earlier paper [Trans. Amer. Math. Soc. **105** (1962), 359–371], the author gave a necessary and sufficient condition on a sequence $\{b_n\}$ of complex numbers in order that there exist a function f in $K(C)$ such that $\mathcal{L}_n(f)=b_n(n=0, 1, 2, \ldots)$. In the present paper, it is shown that the hypothesis that C be convex is not needed. Certain cases are then shown in which if C is taken as large as possible, then it is not convex, so that the new form of the theorem is necessary. A theorem concerning Lidstone functionals which is an improvement of another theorem in the earlier paper is also stated.

Cavity resonances for spherical earth with a concentric anisotropic shell, J. R. Wait, *J. Atmos. Terrest. Phys.* **27,** *81–89 (1965).*

A boundary-value problem of a concentric spherical system involving anisotropic media is considered. Rather gross simplifications are made in order to achieve tractability and yield physical insight. The principal idealization is the representation of the concentric plasma layer by a thin shell of ionization. The derived results have some relevance to the phenomenon of resonance in the concentric cavity formed by the earth and the ionosphere. For example, it is shown that the earth's magnetic field and the electron collisions both contribute to the damping of the cavity resonances.

A method for the computation of the error function of a complex variable, O. N. Strand, *Math. Comp.* **XIX,** *No. 89, 127–129 (Jan. 1965).*

This paper presents a method of computing $\operatorname{erf} z = \frac{2}{\sqrt{\pi}} \int_0^z e^{-u^2}\, du$, where z is complex. It is shown that $\operatorname{erfc} z = 1 - \operatorname{erf} z$ has no zeros in the right half plane. An estimate of $|\operatorname{erfc} z|$ is derived.

Bounds for class numbers, M. Newman, *Proc. Pure Mathematics,* Vol. **III.** Theory of Numbers, pp. 70–77 (Am. Math. Soc., 1965).

Bounds for the class number h of algebraic number fields of degree n over the rationals are derived, in terms of the discriminant d of the field. For example it is shown that

$$h < e\{1^{n-2}\sigma(1)+2^{n-2}\sigma(2)+\ldots+\delta^{n-2}\sigma(\delta)\},$$

where $\delta < |\sqrt{d}|$.

Distribution of Student's t in samples from a rectangular universe, M. M. Siddiqui, *Rev. Intern. Stat. Inst.* **32,** *No. 3, 242–250 (1964).*

The distribution of Student's t statistic for samples of sizes two and three from a rectangular universe have been obtained by Rider (Biometrika **21,** (1929), pp. 124–143) and Perlo (Biometrika **25,** (1933), pp. 203–204) respectively by the application of a geometrical method. For a sample of size N the evaluation of $P(|t| \geq t_0)$ is essentially equivalent to the evaluation of the $(N-1)$-volume of the intersection of an N-cone and a side of the N cube. In this paper, using this method, the distribution of t is obtained for samples of size 4, and bounds on $P(|t| \geq t_0)$ are evaluated for samples of sizes 2 to 7 corresponding to 5%, 1% and 0.1% values of classical Student's distribution.

Other NBS Publications

J. Res. NBS 69A (Phys. and Chem.), No. 4 (July–Aug. 1965), 70 cents.

Correlation of successive atomic steps in crystals by relaxation mode analysis. A. D. Franklin. (See above abstracts.)

Reduction of crystallographic point groups to subgroups by homogeneous stress. H. S. Peiser and J. B. Wachtman, Jr.

Effect of hydrostatic pressure on the refractive indices of some solids. R. M. Waxler and C. E. Weir.

Crystallization kinetics and polymorphic transformations in polybutene-1. J. Powers, J. D. Hoffman, J. J. Weeks, and F. A. Quinn, Jr.

Compliance-time-temperature relationships from indentation measurements on a pure-gum rubber vulcanizate. F. L. Roth, G. W. Bullman, and L. A. Wood.

Distribution function of the end-to-end distances of linear polymers with excluded volume effects. J. Mazur. (See above abstracts.)

An additivity rule for the vapor pressure lowering of aqueous solutions. R. A. Robinson and V. E. Bower.

Franck-Condon factors to high vibrational quantum numbers V: O_2 band systems. R. W. Nicholls.

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Matrices of spin-orbit interaction in the electron configurations p^2d and p^4d. J. L. Tech and R. H. Garstang.

Heat of formation of calcium aluminate tricarbonate at 25 °C. H. A. Berman.

Vapor pressure and heat of sublimation of tungsten. R. Szwarc, E. R. Plante, and J. J. Diamond.

Heat capacity and enthalpy measurements on aluminum carbide (Al_4C_3) from 15 to 1173 °K. Thermodynamic properties from 0 to 2000 °K. G. T. Furukama, T. B. Douglas, W. G. Saba, and A. C. Victor.

Properties of aqueous mixtures of pure salts: thermodynamics of the ternary system water-potassium chloride-barium chloride at 25 °C. R. A. Robinson and V. E. Bower.

A wide-range (up to 10^{10} P) rotating cylinder viscometer. A. Napolitano, P. B. Macedo, and E. G. Hawkins.

Internal friction in ZrO_2 containing CaO. J. B. Wachtman, Jr., and W. C. Corwin.

Splitting of equivalent points in noncentrosymmetric space groups into subsets under homogeneous stress. H. S. Peiser, J. B. Wachtman, Jr., F. A. Munley, and L. C. McCleary.

Inclusion of perfluoromethyl groups in the lattice of copolymers of tetrafluoroethylene and hexafluoropropylene. L. H. Bolz and R. K. Eby.

J. Res. NBS 69C (Eng. and Instr.), No. 3 (July-Sept. 1965), 75 cents.

Two-terminal dielectric measurements up to 6×10^8 Hz. M. G. Broadhurst and A. J. Bur.

Improved ten-picofarad fused silica dielectric capacitor. R. D. Cutkosky and L. H. Lee.

Errors in the series-parallel buildup of four-terminal resistors. C. H. Page. (See above abstracts).

Centerable rotator for measuring properties of crystals. C. P. Saylor and H. B. Lowey.

Equipment for single-crystal growth from the melt suitable for substances with a low melting point. A. T. Horton and A. R. Glasgow.

Phase and amplitude contrast microscopy in partially coherent light. M. De and P. K. Mondal.

Exposure time relations for Kossel microdiffraction photographs. H. Yakowitz and D. L. Vieth.

Cartesian diver as a density comparator. H. A. Bowman and R. M. Schoonover.

Cryogenic behavior of selected magnetic materials. J. J. Gniewek and E. Ploge.

J. Res. NBS 69C (Eng. and Instr.), No. 4 (Oct.–Dec. 1965), 75 cents.

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Radio Sci. J. Res. NBS/USNC–URSI, 69D, No. 7 (July 1965), $1.00.

International comparison of atomic frequency standards via VLF radio signals. A. H. Morgan, E. L. Crow, B. E. Blair.
Control of WWV and WWVH standard frequency broadcasts by VLF and LF signals. B. E. Blair and A. H. Morgan.
Measurements of the total electron content and the equivalent slab thickness of the midlatitude ionosphere. R. V. Bhonsle, A. V. da Rosa, and O. K. Garriott.
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Theory of coil antennas. Trilochan Padhi. (See above abstracts.)
Small prolate spheroidal antenna in a dissipative medium. R. H. Williams, R. D. Kelly, and W. T. Cowan.
Calculated curves for groundwave propagation over inhomogeneous earth with pronounced topographical features. K. Furutsu.

Radio Sci. J. Res. NBS/USNC–URSI 69D, No. 8 (Aug. 1965), $1.00.

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Regular Contributions

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Comments on a paper "Measurement of the phase velocity of VLF propagation in the earth ionosphere waveguide" by F. K. Steele and C. J. Chilton. H. F. Bates.
Reply to H. F. Bates' Comments on "Measurement of the phase velocity of VLF propagation in the earth ionosphere waveguide" by F. K. Steele and C. J. Chilton. F. K. Steele and C. J. Chilton.

Radio Sci. J. Res. NBS/USNC–URSI 69D, No. 9 (Sept. 1965), $1.00.

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Magneto-ionic propagation in inhomogeneous media. Part II. Oblique propagation. B. K. Banerjea.
Editorial comment on the scientific papers of Lord Rayleigh (John William Strutt). J. R. Wait.

Radio Sci. J. Res. NBS/USNC–URSI 69D, No. 10 (Oct. 1965), $1.00.

Irreversible power and radiation resistance of antennas in anisotropic ionized gases. K. S. H. Lee and C. H. Papas.
Scattering resonances of a cylindrical plasma. W. M. Leavens.
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Influence of finite ground conductivity on the propagation of VLF radio waves. J. R. Wait and K. P. Spies.
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Radio Sci. J. Res. NBS/USNC–URSI 69D, No. 11 (Nov. 1965), $1.00.

Propagation of pulses in dispersive media. J. R. Wait.
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Atmospheric breakdown limitations to optical maser propagation. R. G. Tomlinson.
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Propagation in a model terrestrial waveguide of nonuniform height theory and experiment. E. Bahar and J. R. Wait.
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The path integrals of LF/VLF wave hop theory. L. A. Berry and M. E. Chrisman.

Reactive loading of arbitrarily illuminated cylinders to minimize microwave backscatter. K-M. Chen.

On the statistical theory of electromagnetic waves in a fluctuating medium (II) Mathematical basis of the analogies to quantum field theory (a digest). K. Furutsu.

Ionospheric radio propagation, K. L. Davies, NBS Mono. 80 (Apr. 1965), $2.75.

Effects of thermal shrinkage on built-up roofing, W. C. Cullen, NBS Mono. 89 (Mar. 4, 1965), 10 cents.

Automatic indexing: A state-of-the-art report, M. E. Stevens, NBS Mono. 91 (Mar. 30, 1965), $1.50.

The examination of weighing equipment, M. W. Jensen and R. W. Smith, NBS Handbook 94 (Mar. 1, 1965), $3.00. (Supersedes H37).

Examination of liquefied petroleum gas liquid-measuring devices, M. W. Jensen, NBS Handb. 99 (Apr. 23, 1965), 35 cents.

Standard frequency and time services of the National Bureau of Standards, NBS Misc. Publ. 236 (Jan. 15, 1965), 15 cents. (Supersedes editions of Dec. 1, 1960 and July 1, 1961).

Standard Reference Materials: Accuracy of solution x-ray spectrometric analysis of copper-base alloys, R. Alvarez and R. Flitsch, NBS Misc. Publ. 260–5 (Mar. 15, 1965), 25 cents.

Systems engineering in ceramics. Proceedings of a symposium April 19, 1964, NBS Misc. Publ. 267 (May 1, 1965), $2.00.

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Transmission loss predictions for tropospheric communication circuits. P. L. Rice, A. G. Longley, K. A. Norton, and A. P. Barsis, NBS Tech. Note 101, Vol. II (May 7, 1965), $1.00.

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Practical aspects of the use of AC-DC transfer instruments, E. S. Williams, NBS Tech. Note 257 (Mar. 9, 1965), 15 cents.

Research on crystal growth and characterization at the National Bureau of Standards July to December 1964, ed. H. F. McMurdie, NBS Tech. Note 260 (May 8, 1965), 50 cents.

Summary of current research on archival microfilm, C. S. McCamy and C. I. Pope, NBS Tech. Note 261 (Apr. 16, 1965), 25 cents.

Bibliograph of fading on microwave line of sight tropospheric propagation paths and associated subjects, H. T. Dogherty, NBS Tech. Note 302 (Aug. 31, 1964), 60 cents.

Studies of solar flare effects and other ionospheric disturbances with a high frequency Doppler technique, V. Agy, D. M. Baker, and R. M. Jones, NBS Tech. Note 306, (Apr. 28, 1965), 75 cents.

Phase and amplitude diversity in over-water transmissions at two microwave frequencies, H. B. Janes, A. W. Kirkpatrick, D. M. Waters, and D. Smith, NBS Tech. Note 307 (Apr. 12, 1965), 40 cents.

Data reduction for stable auroral red arcs observed at Rapid City, South Dakota, J. E. Cruz, R. Davies, L. K. Droppleman, E. Marovich, L. R. Megill, M. H. Rees, L. Reisbeck, and F. E. Roach, NBS Tech. Note 308 (May 3, 1965), 50 cents.

A bibliography of experimental saturation properties of the cryogenic fluids, N. A. Olien and L. A. Hall, NBS Tech. Note 309 (Apr. 9, 1965), 60 cents.

Attenuation of the ground wave of a low frequency electromagnetic pulse, J. C. Morgenstern and J. R. Johler, NBS Tech. Note 310 (Apr. 1965), 30 cents.

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Stability of two-phase annular flow in a vertical pipe, S. Jarvis, Jr., NBS Tech. Note 314 (June 7, 1965), 55 cents.

Bibliograph on tropospheric propagation of radio waves, W. Nupen, NBS Tech. Note 304 (Apr. 1, 1965), $2.00.

Atlas of Fourier coefficients of diurnal variation of foF_2 Part II. Distribution of amplitude and phase, W. B. Jones and R. M. Gallet, NBS Tech. Note 305 (Feb. 14, 1965), 60 cents.

A calorimetric determination of the enthalpy of graphite from 1200 to 2600 °K, E. D. West and S. Ishihara, (Proc. 3d Symp. Thermal Physical Properties, Purdue Univ., Lafayette, Ind., Mar. 22–26, 1965), Book, Advances in Thermophysical Properties at Extreme Temperatures and Pressures, pp. 146–151 (American Society of Mechanical Engineers, New York, N.Y., 1965).

Blood: Bone equilibrium in calcium homoeostasis, J. MacGregor and W. E. Brown, Nature **205,** No. 4969, 359–361 (Jan. 23, 1965).

Carbon monoxide on niobium, R. Klein and J. W. Little, Surface Science **2,** 167–176 (North-Holland Publ. Co., Amsterdam, The Netherlands, 1964).

Fracture in corrosive media, H. L. Logan, Book, Fracture of Engineering Materials, ch. 8, pp. 143–161 (American Society for Metals, Metals Park, Ohio, Nov. 1964).

Gas-phase radiolysis of *n*-pentane. A study of the decompositions of the parent ion and neutral excited pentane molecule, P. Ausloos and S. G. Lias, J. Chem. Phys. **41,** No. 12, 3962–3970 (Dec. 15, 1964).

Impedance of sealed nickel-cadmium dry cells, R. J. Brodd and H. J. DeWane, Electrochem. Tech. **3,** No. 1–2, 12–17 (Jan.–Feb. 1965).

Moderation in instrumentation, J. K. Taylor, Science Teacher **32,** No. 3, 18–19 (Mar. 1965).

Pressure-indicator-paste patterns in duplicate dentures made by different processing technics for the same patients, J. B. Woelfel and G. C. Paffenbarger, J. Am. Dental Assoc. **70,** 339–343 (Feb. 1965).

Measurement of radiation dose distributions with photochromic materials, W. E. McLaughlin and L. Chalkley, Radiology, **84,** No. 1, 124–125 (Jan. 1965).

Soil corrosion, W. J. Schwerdtfeger, Enclyclopedia of Electrochemistry, pp. 1068–1071 (Reinhold Publ. Corp., New York, N.Y., March 1965).

Continuous-absorption hygrometry with a pneumatic bridge utilizing critical flow, W. A. Wildhack, T. A. Perls, C. W. Kissinger, and J. W. Hayes (Proc. 1963 Intern. Symp. Humidity and Moisture, Washington, D.C.), Book, Humidity and Moisture. Measurement and Control in Science and Industry. Vol. **1.** Principles and Methods of Measuring Humidity in Gases, Sec. VI, Paper 53, pp. 552–570 (Reinhold Publ. Corp., New York, N.Y., 1965).

Absolute measurement of W for polonium-210 alpha particles in nitrogen, argon, and argon-methane mixture, Z. Bay and F. D. McLernon, Radiation Res. **24,** No. 1, 1–8 (Jan. 1965).

Atomic lifetimes in neon I, J. Z. Klose, Astrophys. J. **141,** No. 2, 814–818 (Feb. 15, 1965).

Radioisotope dilution and its application to the radioassay of Ce^{144}, L. A. Currie, G. M. France, III, and H. L. Steinberg, Intern. J. Appl. Radiation Isotopes **16,** No. 1, 1–8 (Jan. 1965).

Reference buffer solutions for *p*H measurements in 50% methanol. Dissociation constants of acetic acid and dihydrogen phosphate ion from 10 to 40°, M. Paabo, R. A. Robinson, and R. G. Bates, J. Am. Chem. Soc. **87,** 415–418 (1965).

Resins and technics used in constructing dentures, G. C. Paffenbarger, J. B. Woelfel, and W. T. Sweeney, Dental Clinics of North America, pp. 51–262 (W. B. Saunders Co., Philadelphia, Pa., 1965).

Spectra of matrix-isolated NiF_2 and $NiCl_2$, D. E. Milligan, M. E. Jacox, and J. D. McKinley, J. Chem. Phys. **42,** No. 3, 902–905 (Feb. 1965).

The polarographic analysis of titanium (IV)–EDTA complex: Application to paint pigments, H. W. Berger and B. C. Cadoff, Offic. Digest Paint Tech. **37,** No. 480, 28–34 (Jan. 1965).

The structures of anhydrous sodium trimetaphosphate, $Na_3P_3O_9$,

and the monohydrate, $Na_3P_3O_9 \cdot H_2O$, H. M. Ondik, Acta. Cryst. **18,** Part 2, 226–232 (Feb. 1965).

Vacuum ultraviolet photochemistry. VIII. Propylene, D. A. Becker, H. Ikabe, and J. R. McNesby, J. Phys. Chem. **69,** No. 2, 538–542 (Feb. 1965).

A high-speed (milliseconds) method for the simultaneous measurement of enthalpy, specific heat, and resistivity of electrical conductors at high temperatures, A. Cezairliyan (Proc. 3d Symp. Thermophysical Properties, 1965), Book, Advances in Thermophysical Properties at Extreme Temperatures and Pressures, pp. 253–262 (American Society of Mechanical Engineers, New York, N.Y., 1965).

A magnetic amplifier for use with diode logic, E. W. Hogue, IEEE Trans. Commun. Electron. **83,** No. 75, 803–808 (Nov. 1964).

A study of the variation of the surface electrical resistance of lead iodide films with relative humidity at room temperature, F. E. Jones (Proc. 1963 Intern. Symp. Humidity and Moisture, Washington, D.C.), Book, Humidity and Moisture. Measurement and Control in Science and Industry. Vol. **1** Principles and Methods of Measuring Humidity in Gases, Sec. III, Paper 37, pp. 361–365 (Reinhold Publ. Corp., New York, N.Y., 1965).

Comment on the difference between a non-LTE and a pure absorption model for the line-blanketing effect, R. N. Thomas, Astrophys. J. **141,** 333–335 (Jan. 1, 1965).

Description and analysis of the third spectrum of cerium (Ce III), J. Sugar, J. Opt. Soc. Am. **55,** No. 1, 33–58 (Jan. 1965).

Displacement of dislocation images formed in transmission electron microscopy, R. DeWit, J. Appl. Phys. **36,** No. 1, 329–330 (Jan. 1965).

Effect of temperature on the vacuum ultraviolet transmittance of lithium fluoride, calcium fluoride, barium fluoride, and sapphire, A. H. Laufer, J. A. Pirog, and J. R. McNesby, J. Opt. Soc. Am. **55,** No. 1, 64–66 (Jan. 1965).

Elastic constant of single crystal ThO_2 at 25 °C, P. B. Macedo, W. Capps, and J. B. Wachtman, Jr., J. Am. Ceram. Soc. **47,** No. 12, 651 (Dec. 1964).

Electron density measurements in the magnetically confined arc, C. K. McLane, S. Takeda, W. E. Thomas, Jr., and R. C. Thompson, J. Appl. Phys. **36,** No. 2, 327–341 (Feb. 1965).

On the displacement of dislocation images formed in transmission electron microscopy, R. DeWit, J. Appl. Phys. **36,** No. 1, 329–330 (Jan. 1965).

On the relative roles of free volume and activation energy in the viscosity of liquids, P. B. Macedo and T. A. Litovitz, J. Chem. Phys. **42,** No. 1, 245–256 (Jan. 1, 1965).

An investigation of psychrometric measurement techniques in air-conditioning calorimetry, J. C. Davis and P. R. Achenbach (Proc. 1963 Intern. Symp. Humidity and Moisture, Washington, D.C.), Book, Humidity and Moisture. Measurement and Control in Science and Industry. Vol. **2.** Applications, Sec. IV, Paper 37, pp. 303–313 (Reinhold Publ. Corp., New York, N.Y., 1965).

Application of cooled ir detector in an optical system, S. Abramowitz, A. M. Bass and A. E. Ledford, Jr., Appl. Opt. **4,** No. 2, p. 255 (Feb. 1965).

Observation of the products of ionic collision processes and ion decomposition in a linear, pulsed time-of-flight mass spectrometer, R. E. Ferguson, K. E. McCulloch, and H. M. Rosenstock, J. Chem. Phys. **42,** No. 1, 100–106 (Jan. 1, 1965).

Oscillator strengths for lines of Fe I between 2500 and 3200 A, R. B. King, K. H. Olsen, and C. H. Corliss, Astrophys. J. **141,** No. 2, 354–363 (Feb. 15, 1965).

Reaction $^{59}Co(p, \alpha)\,^{56}Fe$, M. Barloutaud, R. S. Caswell, J. Gasteblis, A. G. De Pinho, and J. Quidort (Proc. Intern. Congress Nuclear Physics, Paris, France, July 2–8, 1964), Compt. Rend. Cong. Intern. Phys. Nucleaire II, 717–719 (Centre National de la Recherche Scientifique, Paris, France, 1964).

Screening effects in elastic electron scattering, E. Zeithler and H. Olsen, Phys. Rev. **136,** No. 6A, A1546–A1552 (Dec. 14, 1964).

The intensity and spectral distribution of scattered ratiation from Co^{60} sources, B. Petree and J. C. Humphreys, Radiology **84,** No. 1, 129–130 (Jan. 1965).

The interaction of 350 keV polarized neutrons with oriented Ho^{165} nuclei, R. Wagner, P. D. Miller, T. Tamura, and H. Marshak, Phys. Letters **10,** No. 316–318 (June 15, 1964).

Vapor phase growth kinetics of potassium and mercury crystals, R. L. Parker and S. C. Hardy, Book, Condensation and Evaporation of Solids, Proc. Symp. Condensation and Evaporation of Solids, pp. 649–664 (Gordon & Breech, New York, N.Y., Nov. 1964).

Zeeman filter, D. G. Dessler and W. G. Schweitzer, Jr., J. Opt. Soc. Am. **55,** No. 3, 284–288 (Mar. 1965).

Cosmic noise absorption events at geomagnetically conjugate stations, C. G. Little, E. R. Schiffmacher, H. J. A. Chivers, and K. W. Sullivan, J. Geophys. Res. **70,** No. 3, 639–648 (Feb. 1, 1965).

Fluctuations in a laser beam over 9- and 90-mile paths, W. R. Hinchman and A. L. Buck, Proc. IEEE **52,** No. 3, 305–306 (Mar. 1964).

On the effect of solar disturbances on the low-radiofrequency ionosphere reflection process, J. R. Johler and J. D. Harper, Jr. (North Atlantic Treaty Organization Advisory Group for Aeronautical Research and Development. Avionics Panel. 6th Symp. Ionospheric Research Committee, AGARD., Naples, Italy, 1961), Book, The Effect of Disturbances of Solar Origin on Communications, ed. G. J. Gassman, pp. 303–304 (Pergamon Press, Inc., New York, N.Y., 1963).

Calculation of the temperature of a flat-plate wet surface under adiabatic conditions with respect to the Lewis relation, T. Kusuda (Proc. 1963 Intern. Symp. Humidity and Moisture, Washington, D.C.), Book, Humidity and Moisture. Measurement and Control in Science and Industry, Vol. **1.** Principles and Methods of Measuring Humidity in Gases, Sec. I, Paper 2, pp. 16–32 (Reinhold Publ. Corp., New York, N.Y., 1965).

Clinical behavior of *o*-ethoxybenzoic acid-eugenol-zinc oxide cements, S. Civjan and G. M. Brauer, J. Dental Res. **44,** No. 1, 80–83 (Jan.–Feb. 1965).

Control of relative humidity and temperature in rubber laboratory of National Bureau of Standards, F. L. Roth and R. D. Stiehler (Proc. 1963 Intern. Symp. Humidity and Moisture, Washington, D.C.), Book, Humidity and Moisture. Measurement and Control in Science and Industry. Vol. **2.** Applications, Sec. III, Paper 35, pp. 287–292 (Reinhold Publ. Corp., New York, N.Y., 1965).

A line-formula notation system for coordination compounds, P. M. McDonnell and R. F. Pasternack, J. Chem. Documentation **5,** No. 1, 56–60 (Feb. 1965).

Decyclization of cyclohexene, 4-methylcyclohexene, and 4-vinylcyclohexene in a single-pulse shock tube, W. Tsang, J. Chem. Phys. **42,** No. 5, 1805–1809 (Mar. 1, 1965).

Direct and inert-gas-sensitized radiolysis and photolysis of methane in the solid phase, P. Ausloos, R. E. Rebbert, and S. G. Lias, J. Chem. Phys. **42,** No. 2, 540–548 (Jan. 15, 1965).

Effect of electrical fields and density in the radiolysis of ethane, H. H. Carmichael, R. Gorden, Jr., and P. Ausloos, J. Chem. Phys. **42,** No. 1, 343–351 (Jan. 1, 1965).

Equilibrium pressures of oxygen over MnO_2–Mn_2O_3 at various temperatures, E. M. Otto, J. Electrochem. Soc. **112,** No. 4, 367–370 (Apr. 1965).

Hydrogen atom addition to olefins: Relative rates at the two carbon positions and derived heats of formation of several alkyl radicals, R. D. Kelley, R. Klein, and M. D. Scheer, J. Phys. Chem. **69,** No. 3, 905–908 (Mar. 1965).

Isotopic mixing in CO chemisorbed on tungsten. A kinetic study, T. E. Madey, J. T. Yates, Jr., and R. C. Stern, J. Chem. Phys. **42,** No. 1, 1372–1378 (Feb. 15, 1965).

Some new co-ordination compounds of copper (II) chloride, C. Reimann and G. Gordon, Nature **205,** No. 4974, 902–903 (Feb. 27, 1965).

Standardization of analytical data obtained with silver-silver chloride electrodes in methanol-water solvents, M. Paabo, R. G. Bates, and R. A. Robinson, Anal. Chem. **37,** 462–464 (1965).

Watermarks for papermaking by electroforming, J. P. Young, Tappi **48,** No. 1, 36A–37A (Jan. 1965); Metal Finishing **63,** No. 4, 79–82 (Apr. 1965).

Latensification in radiographic emulsions, W. L. McLaughlin, J. Photo. Sci. **13,** 1–11 (1965).

On the information in a microphotograph, C. S. McCamy, Appl. Opt. **4,** No. 4, 405–411 (Apr. 1965).

Results of National Bureau of Standards corrosion investigation in disturbed and undisturbed soils, M. Romanoff, Proc. Appalachian Underground Short Course, Tech. Bull. 72, pp. 566–589 (West Virginia Univ., Morgantown, West Va., 1965).

Statistical design of experiments, W. J. Youden, Handbook on Metals Engineering-Design, American Society of Mechanical Engineers, ch. 3, Pt. 5, pp. 583–585 (McGraw-Hill Publ. Corp., New York, N.Y., 1965).

Technique for determining spin-lattice relaxation times, G. A.

Candela and R. E. Mundy, Rev. Sci. Instr. **36,** No. 3, 338–342 (Mar. 1965).

Two cases of stress corrosion cracking in copper tubing, H. L. Logan and G. M. Uginsky, Materials Protection **4,** No. 3, 79–80 (May 1965).

Nomograms for computing real, imaginary, and absolute values of vector ratios, H. S. Bowman, Acoust. Soc. Am. **37,** No. 4, 751 (Apr. 1965).

A study of errors in the measurement of microscopic spheres, C. P. Saylor, Appl. Opt. **4,** No. 4, 477–486 (Apr. 1965).

Definition of "ampere" and "magnetic constant," C. H. Page, Proc. IEEE **53,** No. 1, 100–101 (Jan. 1965).

Electromagnetic measurement, H. W. Lance, SPACE/AERONAUTICS Res. Develop. Handb. **42,** No. 4, 199–202 (1964–1965).

A proper accounting of conformation of a polymer near a surface, E. A. DiMarzio, J. Chem. Phys. Phys. **42,** No. 6, 2101–2106 (Mar. 1965).

A test of analytical expressions for the thermal emissivity of shallow cylindrical cavities, F. J. Kelly and D. G. Moore, Appl. Opt. **4,** No. 1, 31–40 (Jan. 1965).

A universal color language, K. L. Kelly, Color Eng. **3,** No. 2, 16–21 (Mar.–Apr. 1965).

Characteristics of the "synchrontron light" from the NBS–180 MeV machine, K. Codling and R. P. Madden, J. Appl. Phys. **36,** No. 2, 380–387 (Feb. 1965).

Dependence of the superconducting transition temperature on carrier concentration in semiconducting $SrTiO_3$, J. F. Schooley, W. R. Hosler, E. Amber, J. H. Becker, M. L. Cohen, and C. S. Koonce, Phys. Rev. Letters 14, No. 9, 305–307 (Mar. 1, 1965).

Direct observation of the optical anisotropy of the holmium nucleus, E. Ambler, E. G. Fuller, and H. Marchak, Phys. Rev. **138,** No. 1B, B117–B126 (Apr. 12, 1965).

Growth layers on ammonium dihydrogen phosphate, J. L. Torgesen and R. W. Jackson, Science **148,** No. 3672, 952–954 (May 14, 1965).

High silica glass, quartz, and vitreous silica, J. S. Laufer, J. Opt. Soc. Am. **55,** No. 4, 458–460 (Apr. 1965).

Influence of paramagnetic resonance on the static susceptibility. Spin-lattice relaxation time of cupric sulfate pentahydrate, G. A. Candela, J. Chem. Phys. **42,** No. 1, 113–117 (Jan. 1, 1965).

Interference patterns in reverberant sound fields. II, R. V. Waterhouse and R. K. Cook, J. Acoust. Soc. Am. **37,** No. 3, 424–428 (Mar. 1965).

Line profiles in the far-uv absorption spectra of the rare gases, U. Fano and J. W. Cooper, Phys. Rev. **137,** No. 5A, A1364–A1379 (Mar. 1, 1965).

Low temperature magnetic transitions in some rare-earth trichlorides, J. C. Eisenstein, R. P. Hudson, and B. W. Mangum, Phys. Rev. **137,** No. 6A, A1886–A1895 (Mar. 15, 1965).

Multichannel resonances in the forward scattering of electrons by helium, G. E. Chamberlain, Phys. Rev. Letters **14,** No. 15, 581–582 (Apr. 12, 1965).

Nonlinear ambipolar diffusion of an isothermal plasma across a magnetic field, E. R. Mosburg, Jr., and K. B. Persson, Phys. Fluids **7,** No. 11, 1829–1833 (Nov. 1964).

Polymorphism in hydrogen iodide, F. A. Mauer, C. J. Keffer, R. B. Reeves, and D. W. Robinson, J. Chem. Phys. **42,** No. 4, 1465–1466 (Feb. 15, 1965).

Stability of traveling waves in lasers, J. A. White, Phys. Rev. **137,** No. 6A, A1651–A1654 (Mar. 15, 1965).

Temperature and mean free path dependence of the Ginzburg-Landau parameter, S. Gygax and R. H. Kropschot, Phys. Letters **12,** No. 1, 7–9 (Sept. 1, 1964).

The measurement of water vapor boundary layers in biological systems with a radio refractometer, D. M. Gates (Proc. 1963 Intern. Symp. Humidity and Moisture, Washington, D.C.), Book, Humidity and Moisture. Measurement and Control in Science and Industry. Vol. **2.** Applications, Sec. I, Paper 5, pp. 33–38 (Reinhold Publ. Corp., New York, N.Y., 1965).

The use of terahertz photobeats for precise velocity-of-light measurement, Z. Bay and H. S. Boyne, Proc. Enrico Fermi International School of Physics: Course No. XXXI Quantum Electronics and Coherent Light 1963, 352–371 (1964).

Two-electron excitation states in helium, R. P. Madden and K. Codling, Astrophys. J. **141,** No. 2, 362–375 (Feb. 15, 1965).

Potential use of passive probing of atmospheric structure by thermal emissions at radio frequencies, B. R. Bean, E. R. Westwater, and R. L. Abbott (Proc. 1963 Intern. Symp. Humidity and Moisture, Washington, D.C.), Book, Humidity and Moisture. Measurement and Control in Science and Industry. Vol. **2,** Applications, Sec. VII, Paper 71, pp. 595–608 (Reinhold Publ. Corp., New York, N.Y., 1965).

Radio refractometry and its potential for humidity studies, R. E. McGavin and M. J. Vetter (Proc. 1963 Intern. Symp. Humidity and Moisture, Washington, D.C.), Book, Humidity and Moisture. Measurement and Control in Science and Industry. Vol. **2,** Applications, Sec. VII, Paper 66, pp. 553–560 (Reinhold Publ. Corp., New York, N.Y., 1965).

The use of the radio refractometer to measure water vapor turbulence, B. R. Bean and R. E. McGavin (Proc. 1963 Intern. Symp. Humidity and Moisture, Washington, D.C.), Book, Humidity and Moisture. Measurement and Control in Science and Industry, Vol. **2,** Applications, Sec. VII, Paper 67, pp. 561–568 (Reinhold Publ. Corp., New York, N.Y., 1965).

Determination of the composition of complexes and their instability constant by calorimetry, I. The cuprocyanide complexes, A. Brenner, J. Electrochem. Soc. **112,** No. 6, 611–621 (June 1965).

Emission spectroscopy, B. F. Scribner and M. Margoshes, Treatise on Analytical Chemistry, ed. I. M. Kolthoff and P. J. Elving, 6, Pt. 1, ch. 64, 3347–3461 (Inter-Science Publ. Inc., New York, N.Y., 1965).

Gas chromotographic determination of the moisture content of grain, E. L. Weise, R. W. Burke, and J. K. Taylor, (Proc. 1963 Intern. Symp. Humidity and Moisture, Washington, D.C.), Book, Humidity and Moisture, ed. A. Wexler, Vol. **IV,** Principles and Methods of Measuring Moisture in Liquids and Solids, ch. 1, p. 3–6 (Reinhold Publ. Corp., New York, N.Y., 1965).

Isotopic fractionation of uranium in sandstone, Powder River Basin, Wyoming, and Slick Rock District, Colorado, J. N. Rosholt, A. P. Butler, E. L. Garner, and W. R. Shields, Econ. Geol. **60,** No. 2, 199–213 (Mar.–Apr. 1965).

Mass spectrum of yttrium chloride vapor, J. D. McKinley, J. Chem. Phys. **42,** No. 6, 2245–2246 (Mar. 15, 1965).

Method of adjusting force constants and its application to H_2O, H_2CO, CH_2Cl, and their deuterated molecules, T. Shimanouchi and I. Suzuki, J. Chem. Phys. **42,** No. 1, 296–308 (Jan. 1, 1965).

On the twilight sodium emission-2. A theoretical model of sodium abundance, M. Gadsden, Ann. Geophys. **20,** No. 4, 383–396 (Oct.–Dec. 1964).

Oxidation of asphalt flux with oxides of nitrogen, P. G. Campbell and J. R. Wright, Ind. Engr. Chem. Prod. Res. Develop. **4,** No. 2, 121–128 (June 1965).

Quenching of the triplet state of acetone and biacetyl by azoalkanes, R. E. Rebbert and P. Ausloos, J. Am. Chem. Soc. **87,** 1847–1852 (May 5, 1965).

Radiation-induced polymerization and other reactions of *n*-perfluoropentadiene-1,4 at high temperature and pressure, D. W. Brown, J. E. Fearn, and R. E. Lowry, J. Polymer Sci. **3,** pt. 2, 1641–1660 (1965).

Strength of fingernails, R. W. Young, S. B. Newman, and R. J. Capott, J. Invest. Dermatol. **44,** No. 5, 358–360 (Dec. 23, 1964).

Vacuum-ultraviolet photolysis of ethane in liquid-nitrogen solution, J. A. Pirog and J. R. McNesby, J. Chem. Phys. **42,** No. 7, 2490–2494 (Apr. 1, 1965).

A miniature helium turbo-expander for cryogenic refrigeration systems, M. T. Norton, (Proc. XI Intern. Congress Refrigeration, Munich, Germany, Aug. 1963), Prog. Refrig. Sci. Technol. **1,** 131–135 (1963)

A simple method for measuring the amount of granular materials in sulfur mortars, C. L. Thompson, Mater. Res. Std. **5,** No. 5, 242–243 (May 1965).

A waveguide noise standard, C. K. S. Miller, W. C. Daywitt, and E. Campbell, (Proc. Intern. Measurements Conf.), Acta IMEKO **3,** 371–382 (1964).

A standard for extremely low values of spectral irradiance, R. Stair, W. B. Fussell, and W. E. Schneider, Appl. Opt. **4,** No. 1, 85–89 (Jan. 1965).

Commerical carbon composition resistors as pressure transducers, C. E. Miller, J. W. Dean, and T. M. Flynn, Rev. Sci. Instr. **36,** 231–232 (Feb. 1965).

Human engineering in the design of a console for the comparison of volt boxes, P. H. Lowrie, Jr., 19th Annual Instr. Soc. Am. Conf. Exhibit, Preprint No. 12.1–3–64, pp. 1–8 (Oct. 12–15, 1964).

Maintenance of maring electronic equipment by personnel not

trained in electronic maintenance, G. Shapiro and G. J. Rogers, Proc. Annual Tanker Conf. American Petroleum Institute, pp. A–1–A–18 (June 1965).

Optical instrumentation for the biologist: Microscopy, J. R. Meyer-Arendt, Appl. Opt. **4,** No. 1, 1–9 (Jan. 1965).

Precision detector for complex insertion ratio measuring systems, C. M. Allred and R. A. Lawton, IEEE Trans. Instr. Meas. **IM–13,** No. 2 & 3, 76–81 (June–Sept. 1964).

Stress corrosion cracking of metals, H. L. Logan, Metals Engr. Quart. 5, No. 2, 32–38 (May 1965).

Thermodynamic properties of neon from 25 to 300 °K between 0.1 and 200 atmospheres, R. D. McCarty and R. B. Stewart, Advances in Thermophysical Properties at Extreme Temperatures and Pressures, pp. 84–97, (Am. Soc. Mech. Engr., New York, N.Y., 1965).

The effect of a fatigue crack on the fatigue strength of an aluminum alloy, J. A. Bennett, Mater. Res. Std. **5,** No. 5, 235–239 (May 1965).

The role of cryogenics in the production of high and ultra-high vacuum, L. O. Mullen and M. J. Hiza, Cryogenics **4,** No. 6, 387–394 (Dec. 1964).

Work function measurements on field emitters with prescribed orientation, J. W. Little, T. E. Madey, and R. Klein, J. Appl. Phys. **36,** No. 4, 1491–1492 (Apr. 1965).

Comment on "The use of transforms to sum array factors," M. T. Ma, IEEE Trans. Ant. Prop. **AP–13,** No. 1, 174 (Jan. 1965).

Mathematical programming models for selection of diets to minimize weighted radionuclide intake, H. J. Bracken, Environmental Health Series: Radiological Health, Public Health Serv. Publ. 999–R–4 (Dept. Health, Education, and Welfare, Washington, D.C., Aug. 1963).

A comparison between the National Bureau of Standards two-pressure humidity generator and the National Bureau of Standards hygrometer, S. Hasegawa, R. W. Hyland, and S. W. Rhodes, (Proc. 1963 Intern. Symp. Humidity and Moisture, Washington, D.C.), Book, Humidity and Moisture, Measurement and Control in Science and Industry, ed. A. Wexler, Vol. **3,** Fundamentals and Standards, ch. 22, pp. 455–459 (Reinhold Publ. Corp., New York, N.Y., 1965).

A pneumatic bridge hygrometer for use as a working humidity standard, L. Greenspan, (Proc. 1963 Intern. Symp. Humidity and Moisture, Washington, D.C.), Book, Humidity and Moisture, Measurement and Control in Science and Industry, ed. A. Wexler, Vol. **3** Fundamentals and Standards, ch 20, pp. 433–443 (Reinhold Publ. Corp. New York, N.Y., 1965).

Letter to the Editor, C. H. Page, Metrologia **1,** No. 2, 73–74 (Apr. 1965).

The evolution of designed experiments, W. J. Youden, Proc. IBM Scientific Computing Symp. Statistics, pp. 59–67 (West Chester County, New York, Sept. 1963).

The international system of units, A. G. McNish, Am. Soc. Quality Control Annual Tech. Conf. Trans., pp. 431–438 (1965).

The NBS standard hygrometer, A. Wexler and R. W. Hyland, (Proc. 1963 Intern. Symp. Humidity and Moisture, Washington, D.C.), Book, Humidity and Moisture, Measurement and Control in Science and Industry, ed. A. Wexler, Vol. **3,** Fundamentals and Standards, ch. 19, pp. 389–431 (Reinhold Publ. Corp., New York, N.Y., 1965).

Adsorption of polymer molecules at low surface coverage, C. A. J. Hoeve, E. A. DiMarzio, and P. Peyser, J. Chem. Phys. **42,** No. 7, 2558–2563 (Apr. 1, 1965).

Characteristics of a Raman laser excited by an ordinary ruby laser, H. Takuma and D. A. Jennings, Proc. IEEE **53,** No. 2, 146–149 (Feb. 1965).

Determination of the probability distribution of the number of secondary electrons, Z. Bay and G. Papp, IEEE Trans. Nuclear Sci. **NS–11,** No. 3, 160 (June 1964); Elec. Commun. **40,** No. 1, 134 (1965).

Drift-free Mossbauer spectrometer, F. C. Ruegg, J. J. Spijkerman, and J. R. DeVoe, Rev. Sci. Instr. **36,** No. 3, 356–359 (Mar. 1965).

Effects of finite heat capacity on spin-lattice relaxation, R. L. Peterson, Phys. Rev. **137,** No. 5A, A1444–A1448 (Mar. 1, 1965).

Elastic constants of cubic lead fluoride at room temperature, J. H. Wasilik and M. L. Wheat, J. Appl. Phys. **36,** No. 3, pt. 1, 791–793 (Mar. 1965).

Elastic resonances in electron scattering from He, Ne, Ar, Kr, Xe, and Hg, C. E. Kuyatt, J. A. Simpson, and S. R. Mielczarek, Phys. Rev. **138,** No. 2A, A385–A399 (Apr 19, 1965)

Electron microscopy and diffraction of synthetic corundum crystals. I. Pure aluminum oxide grown by the Verneuil process, D. G. Barber and N. J. Tighe, Phil. Mag. **11,** No. 111, 495–512 (May 1965).

Electronic energy bands in $SrTiO_3$ and related oxide semiconductors, A. H. Kahn and A. J. Leyendecker, Proc. 1964 Intern. Conf. Physics of Semiconductors, Paris, pp. 33–39 (Physique des Semiconducteurs, Paris, France, 1964).

Ice nucleation by photolyzed silver iodide, G. Burley, Phil. Mag. **10,** 527 (Sept. 1964).

Identification of energy levels of negative ions, U. Fano and J. W. Cooper, Phys. Rev. **138,** No. 2A, A400–A402 (Apr. 19, 1965).

Influence of spin paramagnetism on superconductivity, R. A. Kamper, R. S. Collier, and Y. Ohori, Phys. Rev. **137,** 1A A75–A77 (Jan. 4, 1965).

Interpretation of Ar^+-Ar collisions at 50 keV, U. Fano and W. Lichten, Phys. Rev. Letters **14,** No. 16, 627–629 (Apr. 19, 1965).

Longitude distribution of proton flares, C. S. Warwick, Astrophys. J. **141** No. 2, 500–504 (Feb. 15, 1965).

Mass-spectrometric study of photoionization, II. H_2, HD, and D_2, V. H. Dibeler, R. M. Reese, and M. Krauss, J. Chem. Phys. **42,** No. 6, 2045–2048 (Mar. 15, 1965).

Multiple-band conduction in *n*-type rutile (TiO_2), J. H. Becker and W. R. Hosler, Phys. Rev. **137,** No. 6A, A1872–A1877 (Mar. 15, 1965).

On the behavior of the compressibility along the critical isotherm, S. Y. Larsen and J. M. H. L. Sengers, Advances in Thermophysical Properties at Extreme Temperatures and Pressures, pp. 74–75, (Am. Soc. Mech. Engr., New York, N.Y., 1965).

On the validity of the Lorentz-Lorenz equation near the critical point, S. Y. Larsen, R. D. Mountain, and R. Zwanzig, J. Chem. Phys. **42,** No. 6, 2187–2190 (Mar. 15, 1965).

Plans for proposed new tables of the thermodynamic properties of moist air, J. C. Davis, T. K. Faison, Jr., and P. R. Achenbach, (Proc. 1963 Intern. Symp. Humidity and Moisture, Washington, D.C.), Book, Humidity and Moisture, Measurement and Control in Science and Industry, ed. A. Wexler, Vol. **3,** Fundamentals and Standards, ch. 11, pp. 315–320 (Reinhold Publ. Corp., New York, N.Y., 1965).

Optical quenching of photoconductivity near the band edge in CdS, L. Grabner, Phys. Rev. Letters **14,** No. 14, 551–554 (Apr. 5, 1965).

Polar modes of lattice vibration and polaron coupling constants in rutile (TiO_2), D. M. Eagles, J. Phys. Chem. Solids **25,** No. 11, 1243–1251 (Nov. 1964).

Polaron coupling constants in $SrTiO_3$, D. M. Eagles, J. Phys. Chem. Solids **26,** No. 3, 672 (Mar. 1965).

Pressure dependence of the ihternal field at the ^{59}Co nucleus in a 99.5% Ni–0.5% Co alloy, L. H. Bennett, J. Appl. Phys. **36,** No. 3, pt. 2, 942–943 (Mar. 1965).

Stimulated Brillouin scattering in the off-axis resonator, H. Takuma and D. A. Jennings, Appl. Phys. Letters **5,** 239–241 (Dec. 1964).

Structure of electrodeposited lead dendrites, F. Ogburn, C. Bechtoldt, J. B. Morris, and A. deKoranyi, J. Electrochem. Soc. **112,** No. 6, 574–577 (June 1965).

SU(6) Clebsch-Gordan coefficients for the product 35×56, J. C. Carter, J. J. Coyne, and S. Meshkov, Phys. Rev. Letters **14,** No. 13, 523–526 (Mar. 29, 1965).

The absolute photometry of the zodial light, L. L. Smith, F. E. Roach, and R. W. Owen. Planet, Space Sci. 13, 207–217 (Pergamon Press Ltd., Northern Ireland, 1965).

The correlation of experimental pressure-density-temperature and specific heat data for parahydrogen, H. M. Roder, L. A. Weber, and R. D. Goodwin, (Proc. XI Intern. Congress Refrigeration, Munich, Germany, Aug. 1963), Prog. Refrig. Sci. Technol. **1,** 187–191 (1963).

Transition from resonant to non-resonant line shape in microwave absorption, A. Ben-Reuven, Phys. Rev. Letters **14,** No. 10, 349–351 (Mar. 8, 1965).

X-ray spectrochemical analysis of material: cement and dental alloys, B. L. Bean and B. W. Mulligan, Am. Soc. Testing Mater. Spec. Tech. Publ. 373, Application of Advanced and Nuclear Physics to Testing Materials, pp. 25–45 (June 17, 1965).

Measurement and standardization of LF to UHF electrical quantities. Sketch of recent world-wide developments, M. C. Selby, Prog. Radio Sci. 1960–1963, Vol. **1,** Radio Standards and Measurements, pp. 45–55 (Elsevier Publ. Co., Amsterdam, The Netherlands, 1965).

Radio meteorology, J. W. Herbstreit, Science **147,** No. 3653, 76–78 (Jan. 1, 1965).

Stratospheric moisture measurements using infrared spectroscopy,

D. M. Gates, (Proc. 1963 Intern. Symp. Humidity and Moisture, Washington, D.C.), Book, Humidity and Moisture Measurement and Control in Science and Industry, Vol. **2,** Applications, Sec. VI, pp. 446–449 (Reinhold Publ., Corp., New York, N.Y., 1965).

The use of electromagnetic signals emitted from nuclear explosions to study long-range VLF propagation, A. G. Jean and J. R. Wait, J. Geophys. Res. **70,** No. 5, 1258–1261 (Mar. 1, 1965).

The uses of oblique ionograms in frequency utilization, K. Davies, ITU Telecommun. J. **31,** No. 10, pp. 1–7 (Oct. 1964).

Tropospheric propagation, P. L. Rice and J. W. Herbstreit, Advan. Electron. Electron Phys. **20,** 199–259 (1964).

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U. S. GOVERNMENT PRINTING OFFICE : 1966 O-L - 789-972

UNIVERSITY MICROFILMS, INC.
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JOURNAL OF RESEARCH of the National Bureau of Standards Vol. 69B, No. 4 October–December 1965
B. Mathematics and Mathematical Physics

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Library of Congress Catalog Card Number: 62–4414

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402. Price 75 cents (single copy). Subscription price: $2.25 a year, $0.50 additional for foreign mailing.
UNITED STATES GOVERNMENT PRINTING OFFICE, WASHINGTON : 1965